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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Feb 24	PCTGEN now available on STN
NEWS 4	Feb 24	TEMA now available on STN
NEWS 5	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 6	Feb 26	PCTFULL now contains images
NEWS 7	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 8	Mar 24	PATDPAFULL now available on STN
NEWS 9	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 10	Apr 11	Display formats in DGENE enhanced
NEWS 11	Apr 14	MEDLINE Reload
NEWS 12	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 13	AUG 22	Indexing from 1927 to 1936 added to records in CA/CAPLUS
NEWS 14	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 15	Apr 28	RDISCLOSURE now available on STN
NEWS 16	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 17	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 18	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 19	May 19	Simultaneous left and right truncation added to WSCA
NEWS 20	May 19	RAPRA enhanced with new search field, simultaneous left and right truncation
NEWS 21	Jun 06	Simultaneous left and right truncation added to CBNB
NEWS 22	Jun 06	PASCAL enhanced with additional data
NEWS 23	Jun 20	2003 edition of the FSTA Thesaurus is now available
NEWS 24	Jun 25	HSDB has been reloaded
NEWS 25	Jul 16	Data from 1960-1976 added to RDISCLOSURE
NEWS 26	Jul 21	Identification of STN records implemented
NEWS 27	Jul 21	Polymer class term count added to REGISTRY
NEWS 28	Jul 22	INPADOC: Basic index (/BI) enhanced; Simultaneous Left and Right Truncation available
NEWS 29	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS 30	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 31	AUG 15	PATDPAFULL: one FREE connect hour, per account, in September 2003
NEWS 32	AUG 15	PCTGEN: one FREE connect hour, per account, in September 2003
NEWS 33	AUG 15	RDISCLOSURE: one FREE connect hour, per account, in September 2003
NEWS 34	AUG 15	TEMA: one FREE connect hour, per account, in September 2003
NEWS 35	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS 36	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS 37	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right

```
                    Truncation
 NEWS 38  AUG 18  Simultaneous left and right truncation added to ANABSTR

 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 11:53:03 ON 27 AUG 2003

=> file registry
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 11:53:15 ON 27 AUG 2003
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STRUCTURE FILE UPDATES:   25 AUG 2003  HIGHEST RN 573649-48-6
DICTIONARY FILE UPDATES:  25 AUG 2003  HIGHEST RN 573649-48-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09876883.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
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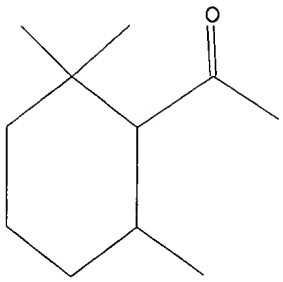

Structure attributes must be viewed using STN Express query preparation.

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=> s l1 sss sam
SAMPLE SEARCH INITIATED 11:53:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1202 TO ITERATE

 83.2% PROCESSED    1000 ITERATIONS                                5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        21961 TO    26119
PROJECTED ANSWERS:               5 TO      267

L2             5 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 11:53:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  23555 TO ITERATE

100.0% PROCESSED   23555 ITERATIONS                            180 ANSWERS
SEARCH TIME: 00.00.01

L3           180 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             148.15     148.36

FILE 'CAPLUS' ENTERED AT 11:54:01 ON 27 AUG 2003
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FILE COVERS 1907 - 27 Aug 2003 VOL 139 ISS 9

FILE LAST UPDATED: 25 Aug 2003 (20030825/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

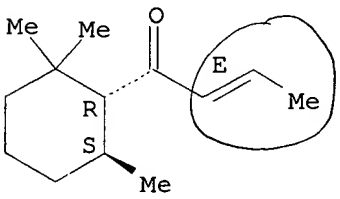
=> s l3
L4 118 L3

=> s l4 and (isomer? or stereoisomer or racemic or cis or trans)
324342 ISOMER?
7995 STEREOISOMER
19420 STEREOISOMERS
24486 STEREOISOMER (STEREOISOMER OR STEREOISOMERS)
29410 RACEMIC
12 RACEMICS
29414 RACEMIC (RACEMIC OR RACEMICS)
192228 CIS
226201 TRANS
5 TRANSES
226205 TRANS (TRANS OR TRANSES)
L5 35 L4 AND (ISOMER? OR STEREOISOMER OR RACEMIC OR CIS OR TRANS)

=> d l5 1-35 hitstr, ibib, iabs

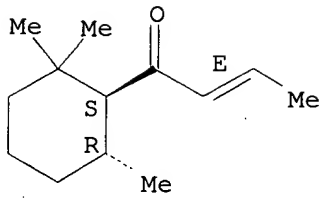
L5 ANSWER 1 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **146726-21-8P 146726-25-2P 379688-80-9P 379688-87-6P**
RL: COS (Cosmetic use); FFD (Food or feed use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and odor of trimethylcyclohexyl ketones via cationic olefin cyclization, stereoselective aldol condensation, and stereoselective oxidn.)
RN 146726-21-8 CAPLUS
CN 2-Buten-1-one, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



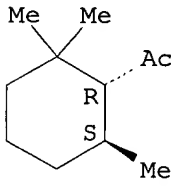
RN 146726-25-2 CAPLUS
CN 2-Buten-1-one, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



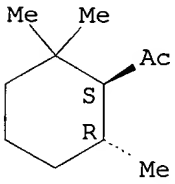
RN 379688-80-9 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



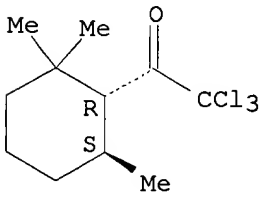
RN 379688-87-6 CAPLUS
CN Ethanone, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **409332-50-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and odor of trimethylcyclohexyl ketones via cationic olefin cyclization, stereoselective aldol condensation, and stereoselective oxidn.)
RN 409332-50-9 CAPLUS
CN Ethanone, 2,2,2-trichloro-1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



Applicant

ACCESSION NUMBER: 2003:28749 CAPLUS
DOCUMENT NUMBER: 138:368540
TITLE: Synthesis and odor of optically active **trans** -2,2,6-trimethylcyclohexyl methyl ketones and their related compounds
AUTHOR(S): Yamamoto, Takeshi; Ujihara, Hideo; Watanabe, Shinya;

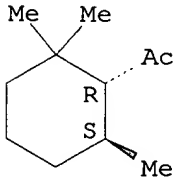
Harada, Makoto; Matsuda, Hiroyuki; Hagiwara, Toshimitsu
CORPORATE SOURCE: Central Research Laboratory, Takasago International Corporation, Hiratsuka, Kanagawa, 254-0073, Japan
SOURCE: Tetrahedron (2003), 59(4), 517-524
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:368540
ABSTRACT:
The syntheses of (1R,6S)-and (1S,6R)-2,2,6-trimethylcyclohexyl Me ketones (I) and (II) via cationic olefin cyclizations of ketone enol esters and their odor is described. (E)-(1R,6S)-and(E)-(1S,6R)-1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one were prepd. via stereoselective aldol condensation of I and II, followed by dehydration. (1R,6S)-Et 2,2,6-trimethylcyclohexylcarboxylate was prepd. via stereoselective oxidn. of I.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Applicant

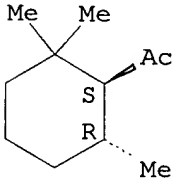
L5 ANSWER 2 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **379688-80-9P**, (1R,6S)-2,2,6-Trimethylcyclohexyl methyl ketone
379688-87-6P, (1S,6R)-2,2,6-Trimethylcyclohexyl methyl ketone
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in perfumes and colognes)
RN 379688-80-9 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



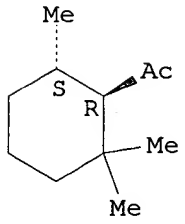
RN 379688-87-6 CAPLUS
CN Ethanone, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



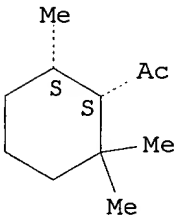
IT **52842-33-8DP**, **trans**-2,2,6-Trimethylcyclohexyl methyl ketone, chiral
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in perfumes and colognes)
RN 52842-33-8 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



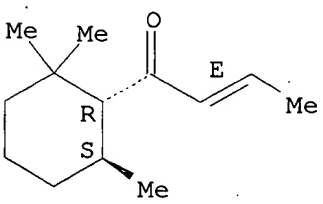
IT **52612-52-9P**, (1S,6S)-2,2,6-Trimethylcyclohexyl methyl ketone
146726-21-8P, **trans**-[(1R,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-22-9P**, **cis**-[(1S,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-23-0P**, **trans**-[(1R,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one **146726-24-1P**, **cis**-[(1S,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one **146726-25-2P**, **trans**-[(1S,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-26-3P**, **cis**-[(1R,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-27-4P**, **trans**-[(1S,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one **146726-28-5P**, **cis**-[(1R,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in perfumes and colognes)
RN 52612-52-9 CAPLUS
CN Ethanone, 1-(2,2,6-trimethylcyclohexyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



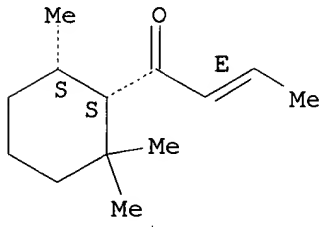
RN 146726-21-8 CAPLUS
CN 2-Buten-1-one, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



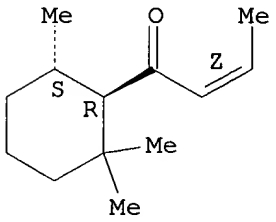
RN 146726-22-9 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(E),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



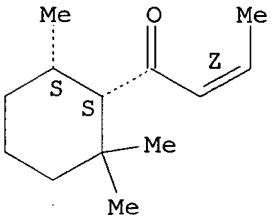
RN 146726-23-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



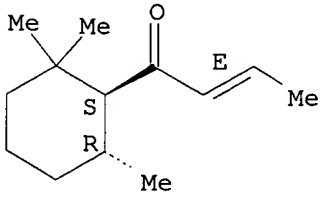
RN 146726-24-1 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



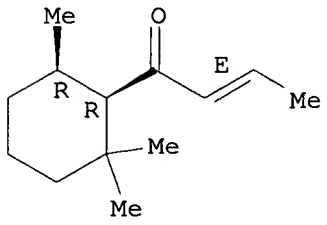
RN 146726-25-2 CAPLUS
CN 2-Buten-1-one, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



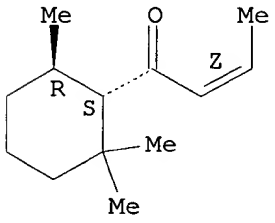
RN 146726-26-3 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(E),6.alpha.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



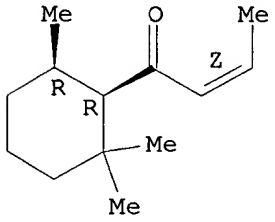
RN 146726-27-4 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.beta.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-28-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.alpha.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

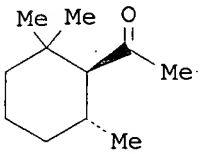


ACCESSION NUMBER:	2001:900121 CAPLUS
DOCUMENT NUMBER:	136:37794
TITLE:	Process for producing (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl methyl ketone and perfume compositions containing them
INVENTOR(S):	Ujihara, Hideo; Watanabe, Shinya; Yamamoto, Takeshi; Toshimitsu, Hagiwara
PATENT ASSIGNEE(S):	Takasago International Corporation, Japan
SOURCE:	Eur. Pat. Appl., 17 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	English

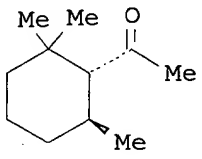
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1162191	A2	20011212	EP 2001-401473	20010607
EP 1162191	A3	20020904		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001348353	A2	20011218	JP 2000-170822	20000607
US 2002042356	A1	20020411	US 2001-876883	20010607

PRIORITY APPLN. INFO.: JP 2000-170822 A 20000607
OTHER SOURCE(S): CASREACT 136:37794
GRAPHIC IMAGE:



I

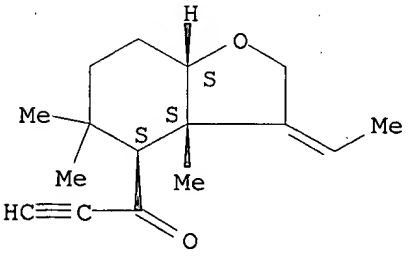


II

ABSTRACT:
A process for producing **trans**-2,2,6-trimethylcyclohexyl Me ketone, which is the (1S,6R)-2,2,6-trimethylcyclohexyl Me ketone (I) and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone (II), is described. Thus, I was prepd. from (R)-citronellol via condensation with EtMgBr in THF, Jones oxidn. in MeCOMe, acetylation with isopropenyl acetate contg. p-MeC6H4SO3H and cyclization with 85% H3PO4 in PhMe. A unique, novel eucalyptus, mint-like and white floral perfume material can be provided using the ketone compds. disclosed in the present invention as well by the prodn. process disclosed therein.

L5 ANSWER 3 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **190852-91-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(radical approaches of the AB ring system and formal synthesis of (.+-.)-forskolin)
RN 190852-91-6 CAPLUS
CN 2-Propyn-1-one, 1-(3-ethylideneoctahydro-3a,5,5-trimethyl-4-benzofuranyl)-, (3a.alpha.,4.alpha.,7a.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



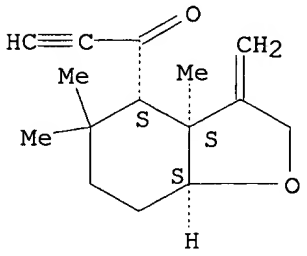
IT **190852-94-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(radical approaches of the AB ring system and formal synthesis of (.+-.)-forskolin)

RN 190852-94-9 CAPLUS

CN 2-Propyn-1-one, 1-(octahydro-3a,5,5-trimethyl-3-methylene-4-benzofuranyl)-, (3a.alpha.,4.alpha.,7a.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



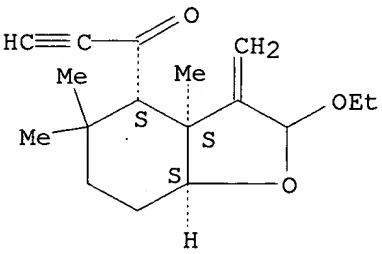
IT **190852-95-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(radical approaches of the AB ring system and formal synthesis of (.+-.)-forskolin)

RN 190852-95-0 CAPLUS

CN 2-Propyn-1-one, 1-(2-ethoxyoctahydro-3a,5,5-trimethyl-3-methylene-4-benzofuranyl)-, (3aR,4R,7aR)-rel-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



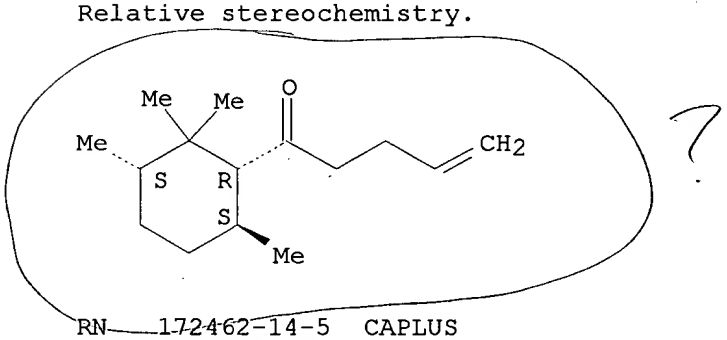
ACCESSION NUMBER: 1997:337845 CAPLUS
DOCUMENT NUMBER: 127:34381
TITLE: A synthetic approach to (.+-.)-forskolin. Part II. Radical approaches of the AB ring system and formal synthesis of (.+-.)-forskolin
AUTHOR(S): Anies, Claude; Pancrazi, Ange; Lallemand, Jean-Yves; Prange, Thierry
CORPORATE SOURCE: Laboratoire de synthese organique associe au CNRS, DCSO, Ecole polytechnique, Palaiseau, 91128, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1997), 134(2), 203-222
CODEN: BSCFAS; ISSN: 0037-8968
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:34381
GRAPHIC IMAGE:

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

ABSTRACT:
A 6-endo-trig cyclization was performed from enynes I (R = OH, R1 = H; RR1 = O) with Bu3SnH/AIBN, leading to the construction of the **trans**-decalinic AB ring system of (.+-.)-forskolin. The diol II was oxidized to its dialdehyde in the second radical approach to (.+-.)-forskolin. A pinacolic coupling reaction of the dialdehyde promoted by SmI2 gave the cyclized 6.beta.,7.beta.-diol III. The unsatd. lactone IV was prepd. from III leading to a formal synthesis of (.+-.)-forskolin.

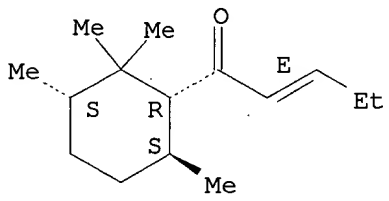
L5 ANSWER 4 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **172462-13-4P 172462-14-5P 172462-15-6P**
172462-17-8P 172462-18-9P 172462-22-5P
172462-23-6P 172462-24-7P 172462-25-8P
172462-26-9P 172462-27-0P 172462-28-1P
172462-29-2P 172586-25-3P 172586-26-4P
172586-27-5P 172586-28-6P 172586-29-7P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of 1-cyclohex(en)ylalkan- and -en-1-ones as perfume fragrances)
RN 172462-13-4 CAPLUS
CN 4-Penten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



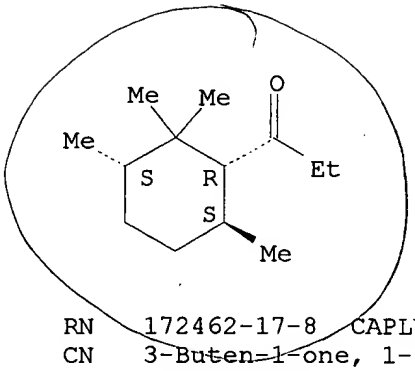
RN 172462-14-5 CAPLUS
CN 2-Penten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, [1.alpha.(E),3.alpha.,6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



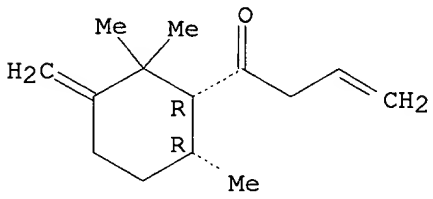
RN 172462-15-6 CAPLUS
CN 1-Propanone, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



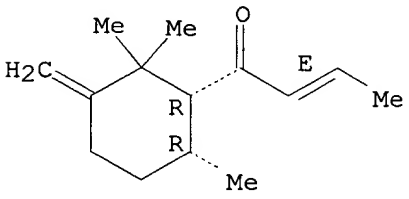
RN 172462-17-8 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

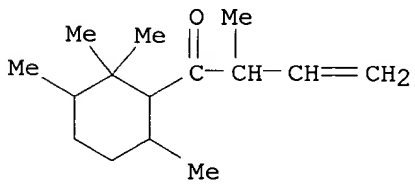


RN 172462-18-9 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, [1.alpha.(E),6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

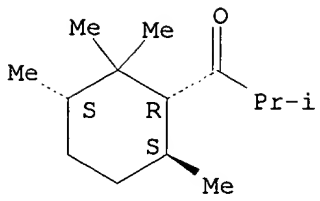


RN 172462-22-5 CAPLUS
CN 3-Buten-1-one, 2-methyl-1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



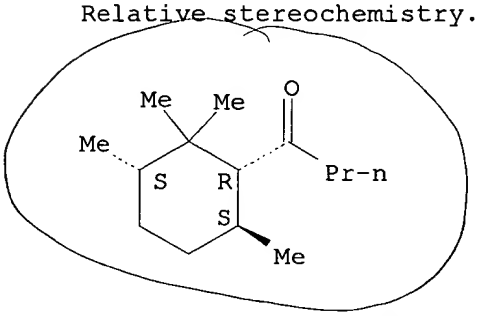
RN 172462-23-6 CAPLUS
CN 1-Propanone, 2-methyl-1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

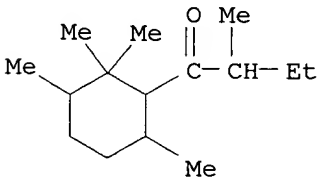


RN 172462-24-7 CAPLUS
CN 1-Butanone, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

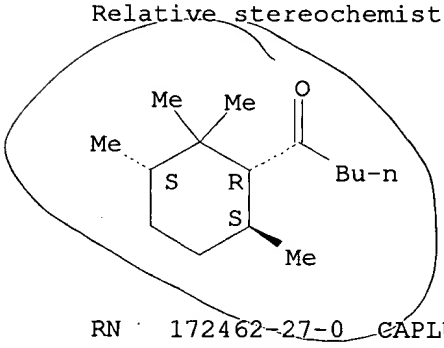


RN 172462-25-8 CAPLUS
CN 1-Butanone, 2-methyl-1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



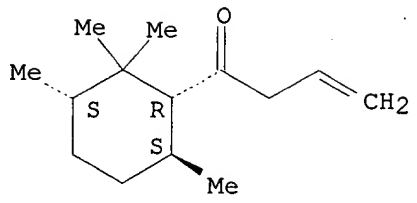
RN 172462-26-9 CAPLUS
CN 1-Pentanone, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



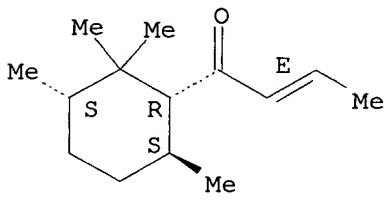
RN 172462-27-0 CAPLUS
CN 3-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



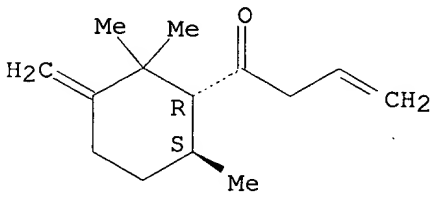
RN 172462-28-1 CAPLUS
CN 2-Buten-1-one, 1-[(1R,3S,6S)-2,2,3,6-tetramethylcyclohexyl]-, (2E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



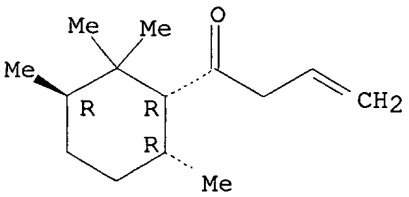
RN 172462-29-2 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



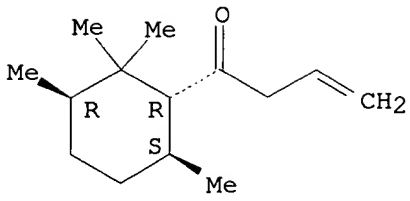
RN 172586-25-3 CAPLUS
CN 3-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.beta.,6.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



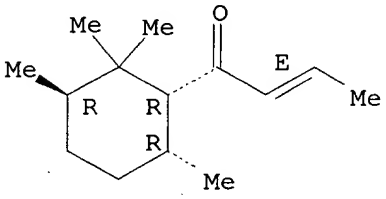
RN 172586-26-4 CAPLUS
CN 3-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



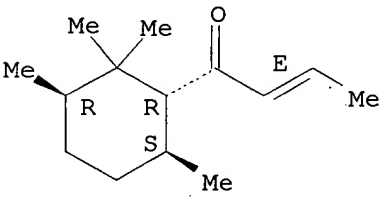
RN 172586-27-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, [1.alpha.(E),3.beta.,6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



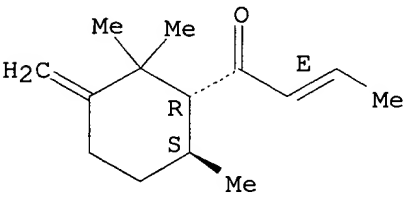
RN 172586-28-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, [1.alpha.(E),3.beta.,6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 172586-29-7 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, [1.alpha.(E),6.beta.]- (9CI) (CA INDEX NAME)

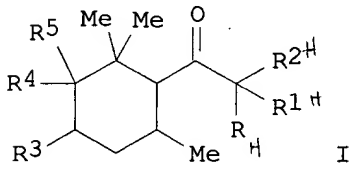
Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1995:994742 CAPLUS
DOCUMENT NUMBER: 124:86432
TITLE: Preparation of 1-cyclohex(en)ylalkan- and -en-1-ones as perfume fragrances
INVENTOR(S): Schulte-Elte, Karl-Heinrich; Chapuis, Christian;

	Pamingle, Herve; Blanc, Pierre-Alain
PATENT ASSIGNEE(S):	Firmenich S. A., Switz.
SOURCE:	Eur. Pat. Appl., 20 pp.
	CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 676393	A1	19951011	EP 1995-103729	19950315
EP 676393	B1	19980819		
R: CH, DE, FR, GB, LI, NL				
PRIORITY APPLN. INFO.:			CH 1994-1047	19940408
OTHER SOURCE(S):	MARPAT 124:86432			
GRAPHIC IMAGE:				



I

ABSTRACT:
Title compds. [I; R = H or Me; R1 = H, alk(en)yl; R2-R4 = H; R1R2 = alkylidene; R3R4 = bond; R5 = Me; R4R5 = CH2] were prepd. Thus, 2,2,3,6-tetramethyl-3-cyclohexene-1-carboxaldehyde was condensed with EtMgBr and the product oxidized to give **cis**-1-(2,2,3,6-tetramethyl-3-cyclohexen-1-yl)-1-propanone. Perfume formulations comprising I were given.

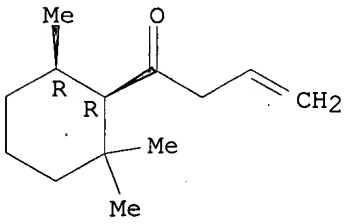
L5 ANSWER 5 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

IT **146726-38-7P 146726-39-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of methylcyclohexylbutenone flavoring agent)

RN 146726-38-7 CAPLUS

CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1R-cis)- (9CI) (CA INDEX NAME)

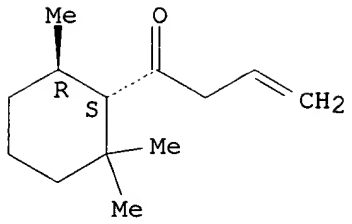
Absolute stereochemistry.



RN 146726-39-8 CAPLUS

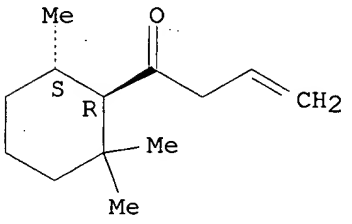
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



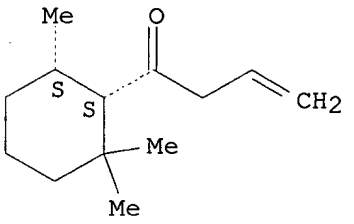
IT **146657-22-9P 146726-32-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of)
RN 146657-22-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



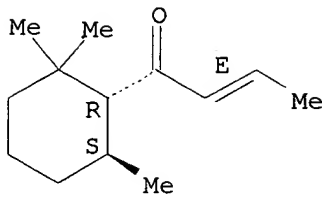
RN 146726-32-1 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



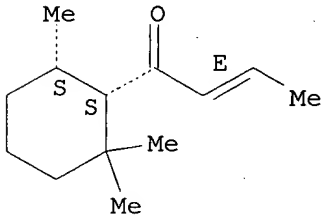
IT **146726-21-8P 146726-22-9P 146726-23-0P**
146726-24-1P 146726-25-2P 146726-26-3P
146726-27-4P 146726-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as flavoring agent)
RN 146726-21-8 CAPLUS
CN 2-Buten-1-one, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



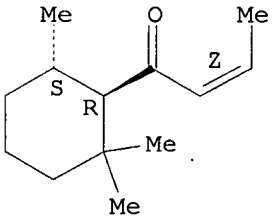
RN 146726-22-9 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(E),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



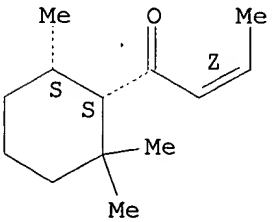
RN 146726-23-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-24-1 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.alpha.]]- (9CI) (CA INDEX NAME)

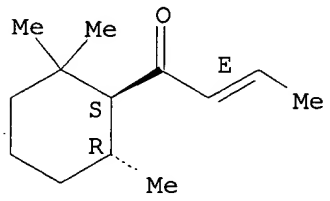
Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-25-2 CAPLUS
CN 2-Buten-1-one, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA

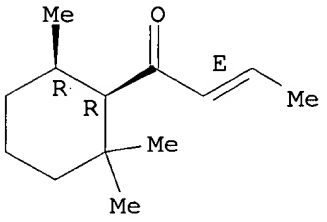
INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



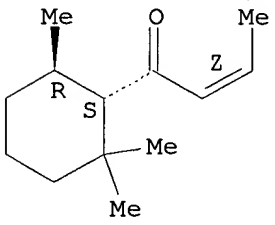
RN 146726-26-3 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(E),6.alpha.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



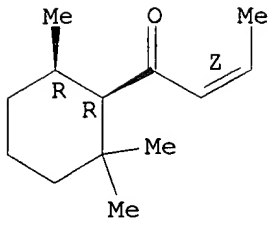
RN 146726-27-4 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.beta.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-28-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.alpha.]]-
(9CI) (CA INDEX NAME)

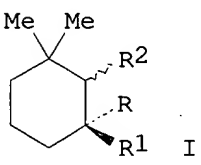
Absolute stereochemistry.
Double bond geometry as shown.



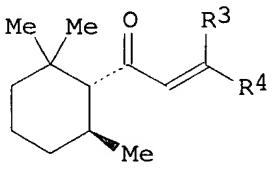
ACCESSION NUMBER: 1993:254447 CAPLUS
DOCUMENT NUMBER: 118:254447
TITLE: Preparation of optically active 1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one compounds as flavor compositions
INVENTOR(S): Shimada, Akiyoshi; Omoto, Tatsuya; Yamamoto, Takeshi
PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04330033	A2	19921118	JP 1990-236980	19900910
JP 2748184	B2	19980506		

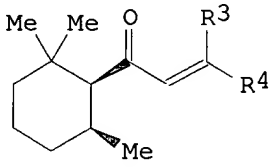
PRIORITY APPLN. INFO.: JP 1990-236980 19900910
OTHER SOURCE(S): CASREACT 118:254447
GRAPHIC IMAGE:



I



II



III

ABSTRACT:
The title compds. (I; R = H, R1 = Me; R = Me, R1 = H; R2 = COCH:CHMe), having fruit-like flavor, are prepd. A flavor compn. contg. I is used for foods, beverages, cosmetics, flavoring agents, and sanitation materials. Thus, (6S)-I (R = H, R1 = Me, R2 = CHO)(prepn. given) 100, allyl bromide 120, Zn powder 83 g, 200 mL DMF were stirred at room temp. for 4 h to give 83% (6S)-I [R = H, R1 = Me, R2 = CH(OH)CH2CH:CH2] as a mixt. **trans**-threo-, **trans**-erythro-, **cis**-threo-, **cis**-erythro-**isomers** which (104 g) was oxidized with Cr3O in aq. acetone contg. H2SO4 at 20-25.degree. to give 91% I (R = H, R1 = Me, R2 = COCH2CH:CH2) contg. 91% **trans**-***isomer*** and 9% **cis**-**isomer**. This (95 g) was heated with 4.8 g p-Me6H4SO3H in PhMe for **isomerization** at 80.degree. for 30 min to give (6S)-I (R = H, R1 = Me, R2 = COCH:CHMe) contg. **trans**-(E)-

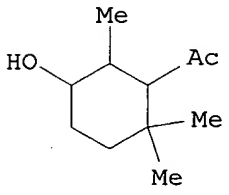
isomer II (R3 = H, R4 = Me) 87.2, **cis**-(E)-**isomer** III (R3 = H, R4 = Me) 8.4, **trans**-(Z)-**isomer** II (R3 = Me, R4 = H) 4.0, and **cis**-(Z)-**isomer** III (R3 = Me, R4 = H) 0.3% which showed strong diffusion property and ripe fruit-like flavor with rose petal-like warm flowery flavor. (6R)-I (R = H, R1 = Me, R2 = COCH:CHMe) was also prepd. and showed a camphor-like flavor as well as a fruit-like flavor with green apple tone, a stimulating green floral tone, or a .beta.-damascone-like tone.

L5 ANSWER 6 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

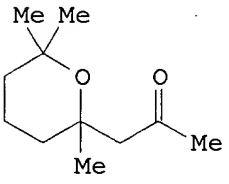
IT **144428-84-2P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in superacid cyclization of dimethylnonadienones)

RN 144428-84-2 CAPLUS

CN Ethanone, 1-(5-hydroxy-2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1992:634262 CAPLUS
DOCUMENT NUMBER: 117:234262
TITLE: Cyclization of acyclic isoprenoids. VI. Cyclization of **trans**- and **cis**-2,6-dimethylnonadienones
AUTHOR(S): Gavrilyuk, O. A.; Korchagina, D. V.; Barkhash, V. A.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, Russia
SOURCE: Zhurnal Organicheskoi Khimii (1992), 28(1), 111-21
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GRAPHIC IMAGE:



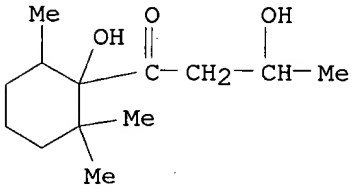
II

ABSTRACT:

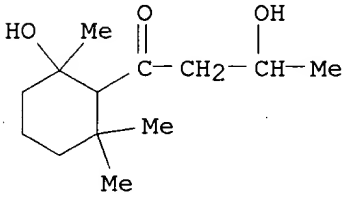
trans- And **cis**-2,6-dimethylnonadienones, e.g. MeCOCH:CMeCH2CH2CH:CMe2 (I), depending on conditions, are cyclized by superacids either by stereoselective heterocyclization process or by an ionic type carbocyclization reaction which does not depend on the geometry of 6,7-double bond in the starting ketones. Thus, **trans**-I and its ***cis*** **isomer** treated with HSO3F-SO2ClF at -90.degree. gave, after cyclization at 20.degree., pyran deriv. II via carbocation intermediates.

L5 ANSWER 7 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

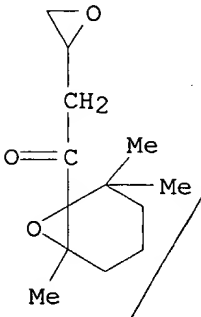
IT **132367-14-7P 132367-15-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydration of)
RN 132367-14-7 CAPLUS
CN 1-Butanone, 3-hydroxy-1-(1-hydroxy-2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 132367-15-8 CAPLUS
CN 1-Butanone, 3-hydroxy-1-(2-hydroxy-2,6,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)

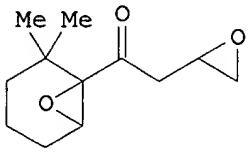


IT **132367-06-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring cleavage of)
RN 132367-06-7 CAPLUS
CN Ethanone, 2-oxiranyl-1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1991:102429 CAPLUS
DOCUMENT NUMBER: 114:102429
TITLE: Photochemical syntheses of .beta.-damascenone and .beta.-damascone
AUTHOR(S): Wu, Guosheng; Hu, Jun; Wu, Biqi; Chen, Zhaobin; Wang, Yinzhang
CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China
SOURCE: Huaxue Xuebao (1990), 48(11), 1113-19

CODEN: HHHPA4; ISSN: 0567-7351
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 114:102429
GRAPHIC IMAGE:

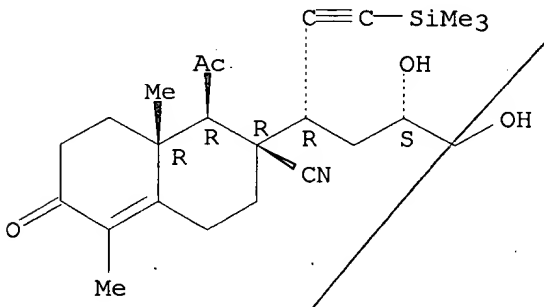


III

ABSTRACT:
.beta.-Damascenone (I) and .beta.-damascone (II) were synthesized from the same intermediate, the bisepoxide III, derived from the photooxidn. of allylic .beta.-cyclogeraniol. Protection of the carbonyl group of III with o-nitrophenyl glycol, redn., photodeprotection and dehydration gave II while I was obtained by means of acid catalytic ring-opening of the epoxy groups of III, protection, redn. and photodeprotection. It was the first time to observe epoxidn. of terminal double bond under photooxidn.

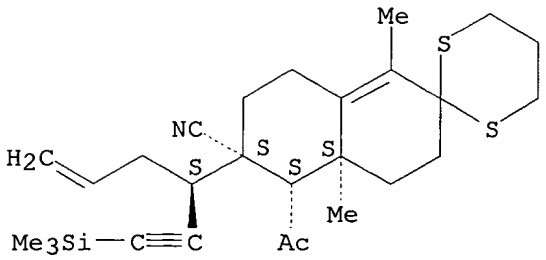
L5 ANSWER 8 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **124800-69-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)
RN 124800-69-7 CAPLUS
CN 2-Naphthalenecarbonitrile, 1-acetyl-2-[3,4-dihydroxy-1-[(trimethylsilyl)ethynyl]butyl]-1,2,3,4,6,7,8,8a-octahydro-5,8a-dimethyl-6-oxo-, [1.alpha.,2.alpha.,2(1R*,3S*),8a.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

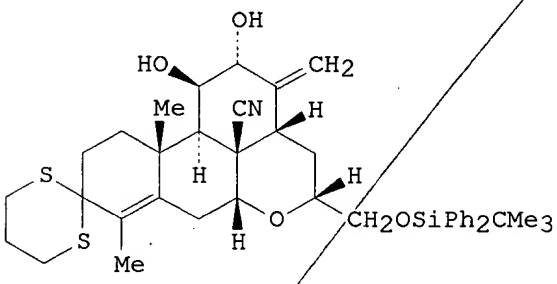


IT **124778-51-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ketal hydrolysis of)
RN 124778-51-4 CAPLUS
CN Spiro[1,3-dithiane-2,2'(3'H)-naphthalene]-6'-carbonitrile, 5'-acetyl-4',4'a,5',6',7',8'-hexahydro-1',4'a-dimethyl-6'-[1-[(trimethylsilyl)ethynyl]-3-butenyl]-, [4'a.alpha.,5'.alpha.,6'.alpha.(R*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



ACCESSION NUMBER: 1990:56354 CAPLUS
DOCUMENT NUMBER: 112:56354
TITLE: An approach to the synthesis of bruceantin. The synthesis of a tetracyclic intermediate
AUTHOR(S): Darvesh, Sultan; Grant, Andrew S.; MaGee, David I.; Valenta, Zdenek
CORPORATE SOURCE: Dep. Chem., Univ. New Brunswick, Fredericton, NB, E3B 6E2, Can.
SOURCE: Canadian Journal of Chemistry (1989), 67(12), 2237-40
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:56354
GRAPHIC IMAGE:

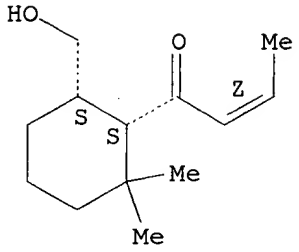


I

ABSTRACT:
An intermediate (I) contg. four of the five rings and seven of the ten chiral centers of bruceantin was prepd. In a key reaction, 3-iodo-1-trimethylsilyl-5-hexen-1-yne added chemoselectively and stereoselectively to a dianion. The sequence also includes a selective attack by a sulfinate on the terminal acetylene C-atom of the dianion of a keto acetylene, a concomitant cyclization in which the acetylene acts as an electrophile, and the use of the resulting allyl sulfoxide for the introduction of O functionality by a reductive rearrangement.

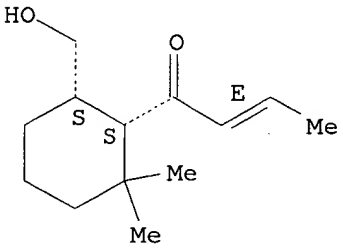
L5 ANSWER 9 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **122291-62-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(byproduct of .beta.-cleavage of (diallyl)cyclohexylcarbanol deriv.)
RN 122291-62-7 CAPLUS
CN 2-Buten-1-one, 1-[6-(hydroxymethyl)-2,2-dimethylcyclohexyl]-, [1.alpha.(Z),6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



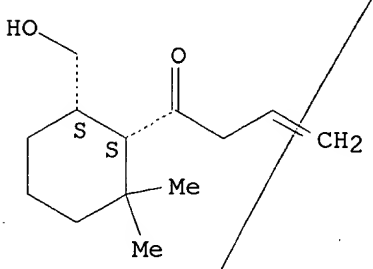
IT **122203-65-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(byproduct of .beta.-cleavage of (diallyl)cyclohexylcarbinol deriv.)
RN 122203-65-0 CAPLUS
CN 2-Buten-1-one, 1-[6-(hydroxymethyl)-2,2-dimethylcyclohexyl]-, [1.alpha.(E),6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



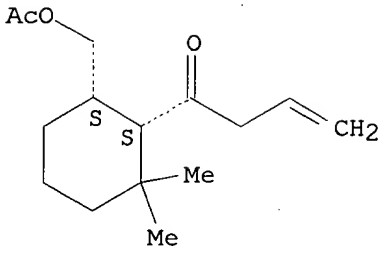
IT **122203-64-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and acetylation of)
RN 122203-64-9 CAPLUS
CN 3-Buten-1-one, 1-[6-(hydroxymethyl)-2,2-dimethylcyclohexyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



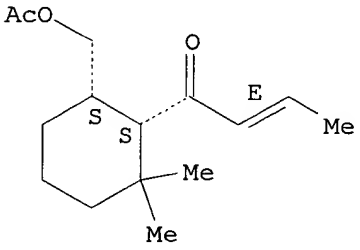
IT **122203-66-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and **isomerization** of)
RN 122203-66-1 CAPLUS
CN 3-Buten-1-one, 1-[6-[(acetyloxy)methyl]-2,2-dimethylcyclohexyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

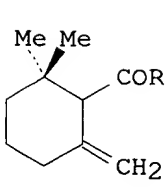


IT **122203-67-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and pyrolysis of)
RN 122203-67-2 CAPLUS
CN 2-Buten-1-one, 1-[6-[(acetyloxy)methyl]-2,2-dimethylcyclohexyl]-, [1.alpha.(E),6.alpha.]- (9CI) (CA INDEX NAME)

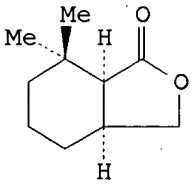
Relative stereochemistry.
Double bond geometry as shown.



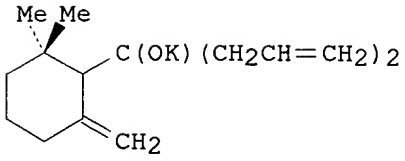
ACCESSION NUMBER:	1989:497527 CAPLUS
DOCUMENT NUMBER:	111:97527
TITLE:	.beta.-Cleavage of bis(homoallylic) potassium alkoxides. Synthesis of .gamma.-damascone
AUTHOR(S):	Snowden, Roger L.; Linder, Simon M.
CORPORATE SOURCE:	Res. Lab., Firmenich S. A., Geneva, CH-1211, Switz.
SOURCE:	Helvetica Chimica Acta (1988), 71(7), 1587-97 CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 111:97527
GRAPHIC IMAGE:	



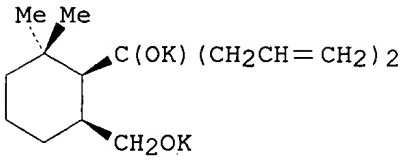
I



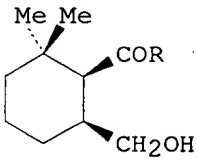
II



III



IV



V

ABSTRACT:
.gamma.-Damascone [I (R = (E)-MeCH:CH)] was prepd. from .gamma.-lactone II via two routes. The key step in each involved the .beta.-cleavage of a bis(homoallylic) potassium alkoxide, namely, the transformations of III to I [R = (E/Z)-MeCH:CH] and I [R = CH2CH:CH2] and of IV to V [R = (E/Z)-MeCH:CH, CH2CH:CH2].

L5 ANSWER 10 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

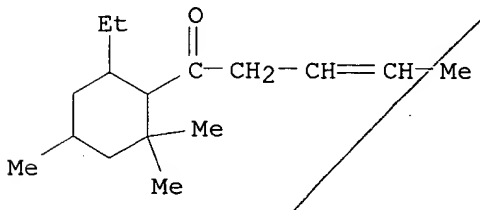
IT **113405-74-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**isomerization** of)

RN 113405-74-6 CAPLUS

CN 3-Penten-1-one, 1-(6-ethyl-2,2,4-trimethylcyclohexenyl)- (9CI) (CA INDEX NAME)

CM 1

CRN 113405-73-5
CMF C16 H28 O



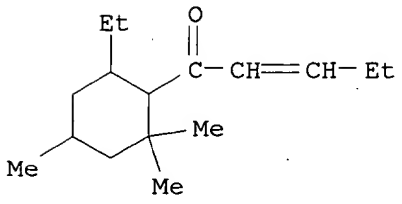
IT **113405-72-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, from alkynol and allyl bromide derivs.)

RN 113405-72-4 CAPLUS

CN 2-Penten-1-one, 1-(6-ethyl-2,2,4-trimethylcyclohexenyl)- (9CI) (CA INDEX NAME)

CM 1

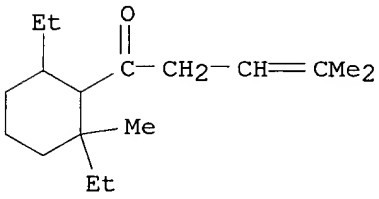
CRN 113405-71-3
CMF C16 H28 O



IT **113405-68-8P 113405-70-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, in synthesis of .alpha.,.beta.-unsatd. alkenoylcyclohexene derivs.)
RN 113405-68-8 CAPLUS
CN 3-Penten-1-one, 1-(2,6-diethyl-2-methylcyclohexenyl)-4-methyl- (9CI) (CA INDEX NAME)

CM 1

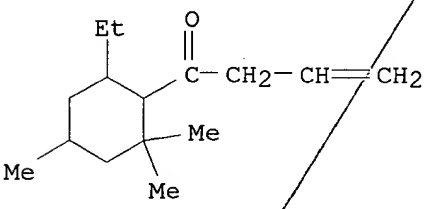
CRN 113405-67-7
CMF C17 H30 O



RN 113405-70-2 CAPLUS
CN 3-Buten-1-one, 1-(6-ethyl-2,2,4-trimethylcyclohexenyl)- (9CI) (CA INDEX NAME)

CM 1

CRN 113405-69-9
CMF C15 H26 O

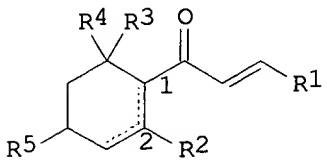


ACCESSION NUMBER: 1988:131103 CAPLUS
DOCUMENT NUMBER: 108:131103
TITLE: Process for the preparation of .alpha.,.beta.-unsaturated alkenoylcyclohexene derivatives
INVENTOR(S): Masso Ortigosa, Maria Teresa
PATENT ASSIGNEE(S): Spain
SOURCE: Span., 23 pp.

CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 542918	A1	19860716	ES 1985-542918	19850508

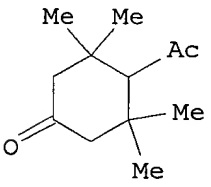
PRIORITY APPLN. INFO.: ES 1985-542918 19850508
GRAPHIC IMAGE:



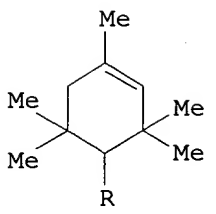
I

ABSTRACT:
Title derivs. I (R1 = H, C1-6 alkyl; R2-R5 = H, Me, Et, Pr) some of which are naturally occurring, are prepd. by a 5-step synthesis: (1) C-alkylation of R3R4C:CHCHR5CH2CR2(OH)C.tplbond.CH with BrCH2CH:CHR1; (2) hydroboration-oxidn. of the triple bond to give R3R4C:CHCHR5CH2CR2(OH)CH2COCH2CH:CHR1; (3) dehydration of the alc. to give the .alpha.,.beta.-unsatd. compd.; (4) cyclization of the 1,5-diene moiety; and (5) **isomerization** of the resultant .beta.,.gamma.-unsatd. alkenoylcyclohexene derivs. Yields for the steps were: (1) 67%; (2) 45-70%; (3) 67.9-87.9%; (4) 84- 93%; and (5) 80%.

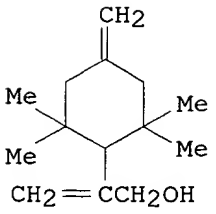
L5 ANSWER 11 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **16556-46-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16556-46-0 CAPLUS
CN Cyclohexanone, 4-acetyl-3,3,5,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1985:406521 CAPLUS
DOCUMENT NUMBER: 103:6521
TITLE: Terpenes and terpenoid compounds, 17. Preparation of oxygenated tetramethylmenthenes and tetramethylmenthadienes
AUTHOR(S): Pauluth, Detlef; Hoffmann, H. M. R.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hannover, Hannover, D-3000, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1985), (4), 756-64
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 103:6521
GRAPHIC IMAGE:



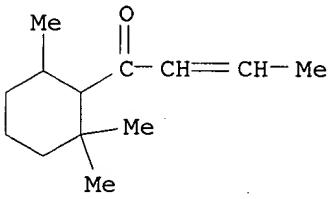
I



$CH_2{=}CCH_2OH$ III

ABSTRACT:
Hydroboration-oxidn. of (.+-.)-tetramethyllimonene (I, R = CMe:CH2) (II) with 9-BBN gave selectively the menthenols I (R = CHMeCH2OH), whereas treatment of II with 9-BBN followed by EtCO2H and p-MeC6H4SO3H gave the tetramethylmenthene I (R = CHMe2). Hydrochlorination of II followed by epoxidn. and treatment with LiN(CHMe2)2 gave the .DELTA.1(7),8-p-menthadienol III, acid catalyzed ***isomerization*** of which gave the .DELTA.1,8-p-menthadienol I [R = C(:CH2)CH2OH].

L5 ANSWER 12 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **39900-18-0D,** derivs.
RL: BIOL (Biological study)
(perfume compns. contg. phenylethyl Me carbonate and)
RN 39900-18-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1984:428113 CAPLUS
DOCUMENT NUMBER: 101:28113
TITLE: Phenylethyl methyl carbonate, mixtures containing it and their organoleptic uses
INVENTOR(S): Boden, Richard M.; Tyszkiewicz, Theodore J.; Watkins, Hugh
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc. , USA
SOURCE: U.S., 14 pp. Division of U.S. Ser. No. 329,221.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

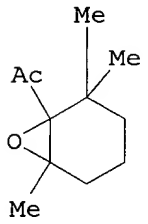
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4436652	A	19840313	US 1982-422489	19820923
US 4464280	A	19840807	US 1983-546390	19831028

PRIORITY APPLN. INFO.: US 1981-329221 19811210
US 1982-422489 19820923

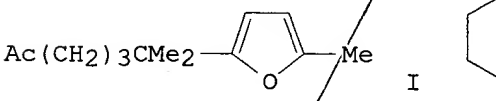
ABSTRACT:
Perfumes and perfumed articles consist of a mixt. of phenylethyl methyl

carbonate (I) [1796-66-3], 5-phenyl-3-methylpentanol **isomers** and 1 or more butenoylcyclohexane derivs. The mixt. may be used in hair sprays, shampoos, cosmetics, etc. Thus, I was prepd. by the condensation of phenylethyl acetate [103-45-7] and (MeO)2CO [616-38-6] in the presence of NaOMe. The use of I along with other ingredients in improving the odor of various formulations is given.

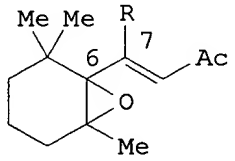
L5 ANSWER 13 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **58254-13-0**
RL: PRP (Properties)
(carbon-13 NMR of, configuration, conformation, and epoxyenone-furan rearrangement mechanism in relation to)
RN 58254-13-0 CAPLUS
CN Ethanone, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



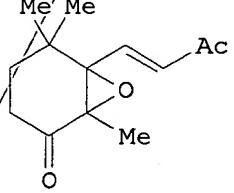
ACCESSION NUMBER: 1984:120184 CAPLUS
DOCUMENT NUMBER: 100:120184
TITLE: Carbon-13 NMR spectroscopy of carbonyl compounds. 2. Conformational and configurational dependence of the (Z)-epoxyenone/furan **isomerization**
AUTHOR(S): Muellen, Klaus; Kotzamani, Eleni; Schmickler, Hans; Frei, Bruno
CORPORATE SOURCE: Inst. Org. Chem., Univ. Koeln, Cologne, D-5000/41, Fed. Rep. Ger.
SOURCE: Tetrahedron (1983), 39(22), 3821-31
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:120184
GRAPHIC IMAGE:



I



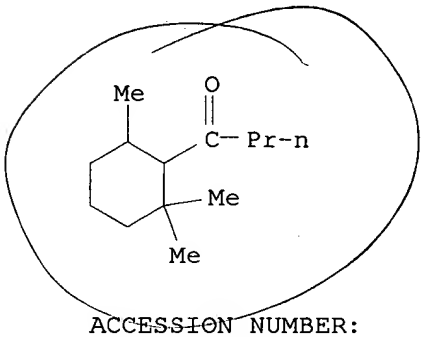
II



IV

ABSTRACT:
The furan deriv. I, isolated upon the photolysis of the epoxyenone (E)-1
H) (III), results from the thermal **isomerization** of III to the (Z)-
isomer . The conversion of III to I is a multicenter process inv
a nucleophilic attack of the CO group O atom upon the oxirane ring. Insp
of related epoxyenones II (R = Me) and IV shows that the ease of rearrang
of the (Z)-epoxyenones to furans depends upon the conformation about the
C(6)-C(7) bond. The conformational properties of epoxyenones and related
dienones and epoxydienes, detd. by dynamic 13C NMR, are used to describe the
epoxyenone/furan rearrangement stereochem.

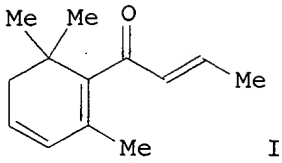
L5 ANSWER 14 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **76038-07-8P**
RL: PREP (Preparation)
(prepn. of, for perfume compns.)
RN 76038-07-8 CAPLUS
CN 1-Butanone, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



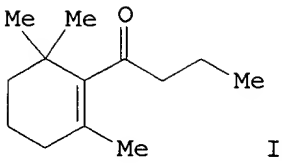
ACCESSION NUMBER: 1981:36129 CAPLUS
DOCUMENT NUMBER: 94:36129
TITLE: Hydrogenation of 2,6,6-trimethyl cyclohexene derivatives for organoleptic uses
INVENTOR(S): Trenkle, Robert Walter; Mookherjee, Braja Dulal; Schmitt, frederick Louis; Vock, Manfred Hugo; Vinals, Joaquin F.; Kiwala, Jacob
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA
SOURCE: Eur. Pat. Appl., 75 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 12436	A1	19800625	EP 1979-105144	19791213
EP 12436	B1	19821124		
R: CH, DE, FR, GB, NL				
US 4292447	A	19810929	US 1978-969852	19781215
US 4311754	A	19820119	US 1981-239051	19810227
US 4313842	A	19820202	US 1981-239049	19810227
US 4315953	A	19820216	US 1981-239048	19810227
US 4324704	A	19820413	US 1981-238680	19810227
US 4360032	A	19821123	US 1981-239052	19810227

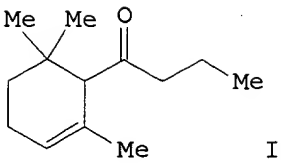
PRIORITY APPLN. INFO.: US 1978-969852 19781215
GRAPHIC IMAGE:



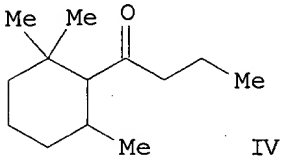
I



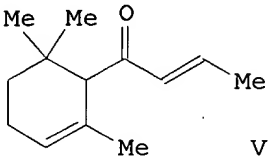
II



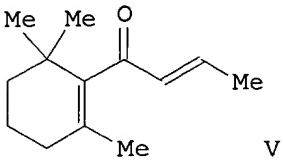
III



IV



V

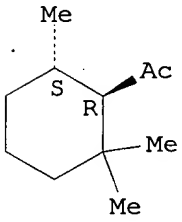


VI

ABSTRACT:
.beta.-Damascenone (I) [23726-93-4] was hydrogenated (H2/Pd/CuCO3) to give a mixt. of II [28384-26-1], III [28361-64-0], and IV [**76038-07-8**]. Using H2/Pd/BaSO4, I gave II, III, V [24720-09-0], and VI [23726-91-2] along with a **cis-isomer** of VI [23726-92-3] as an artifact formed as a result of distn. These fractions from hydrogenation of I were added to perfume compns. to enhance the fragrance note. The perfume compns. were added to soap, detergent, shampoo, hair prepns. and, flavor formulations and as additives for tobacco.

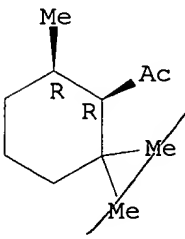
L5 ANSWER 15 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **52842-33-8P 52842-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 52842-33-8 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



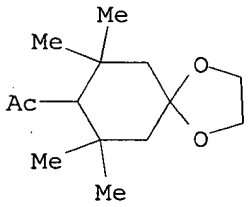
RN 52842-34-9 CAPLUS
CN Ethanone, 1-[(1R,6R)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



ACCESSION NUMBER: 1978:614461 CAPLUS
DOCUMENT NUMBER: 89:214461
TITLE: Reduction of organic compounds with solutions of ytterbium in liquid ammonia
AUTHOR(S): White, James D.; Larson, Gerald L.
CORPORATE SOURCE: Dep. Chem., Oregon State Univ., Corvallis, OR, USA
SOURCE: Journal of Organic Chemistry (1978), 43(23), 4555-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
Solns. of ytterbium in NH3 (l) are stable at -33.degree.C and have powerful reducing properties. Arom. compds. are reduced cleanly to the 1,4-dihydroarom. systems (except durene); thus, estradiol 3-Me ester gave dihydrotestosterone after hydrolysis. .alpha.,.beta.-Unsatd. ketones are reduced to a mixt. of the satd. ketone and corresponding alc. which, after Jones' oxidn., gives ketones in fair-to-good yield; thus, 4-cholesten-3-one gave cholestanone. Alkynes are usually reduced in this medium to **trans**-alkenes; further redn. to the alkane was obsd once. Bicyclo[2.2.1]heptadiene was reduced to bicycloheptene.

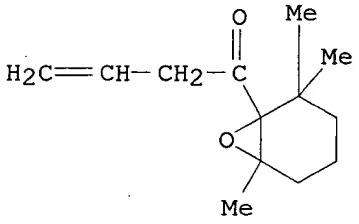
L5 ANSWER 16 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **16556-47-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(redn. of)
RN 16556-47-1 CAPLUS
CN Ethanone, 1-(7,7,9,9-tetramethyl-1,4-dioxaspiro[4.5]dec-8-yl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1977:105786 CAPLUS
DOCUMENT NUMBER: 86:105786
TITLE: Estimation of the stereoselectivity of reduction of 3,3,5,5-tetramethylcyclohexanone by sodium borohydride
AUTHOR(S): Wigfield, Donald C.; Buchanan, Gerald W.; Ashley, Catherine A.; Feiner, Steve
CORPORATE SOURCE: Dep. Chem., Carleton Univ., Ottawa, ON, Can.
SOURCE: Canadian Journal of Chemistry (1976), 54(22), 3536-40
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
4-(1-Hydroxyethyl)-3,3,5,5-tetramethylcyclohexanone was prepd. to serve as a model for 3,3,5,5-tetramethylcyclohexanone on which the redn. stereochem. product ratio may be exptl. detd. Redn. by NaBH4 in Me2CHOH gives 2 epimers in a 95.5:4.5 ratio. The major **isomer** is shown to be the less stable by equilibration over Raney Ni. 1H- and 13C NMR spectra confirm that this major epimer is **cis**-4-(1-hydroxyethyl)-3,3,5,5-tetramethylcyclohexanol and show that this compd. exists predominantly in the conformation with an axial hydroxyethyl group and an equatorial hydroxyl group. Redn. of this model compd. proceeds at least 95.5% by equatorial attack.

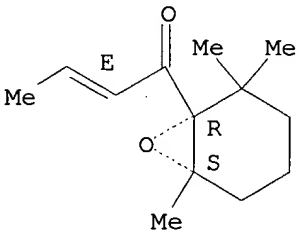
L5 ANSWER 17 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

IT **31089-87-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and **isomerization** of)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



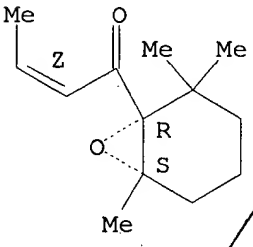
IT **31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1976:446082 CAPLUS
DOCUMENT NUMBER: 85:46082
TITLE: Cycloaliphatic unsaturated ketones as odor- and taste-modifying agents
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich S. A., Switz.

SOURCE: U.S., 34 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

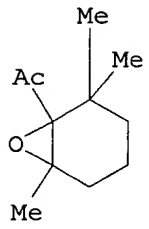
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3928456	A	19751223	US 1974-503794	19740906
CH 498795	A	19701115	CH 1968-498795	19681101
CH 537452	A	19730713	CH 1969-12065	19690808
ES 377485	A1	19720701	ES 1970-377485	19700313
ES 377483	A1	19720701	ES 1970-377483	19700313
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
DD 96077	W	19730312	DD 1970-153631	19700507
US 3975310	A	19760817	US 1974-503738	19740906
US 3931326	A	19760106	US 1974-523743	19741114
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

PRIORITY APPLN. INFO.:

CH 1967-15667	19671109
CH 1968-16309	19681101
US 1968-774179	19681107
CH 1969-6976	19690507
CH 1969-12065	19690808
CH 1970-5559	19700414
CH 1970-5725	19700417
US 1970-35594	19700507
CH 1970-6725	19700417
US 1974-503738	19740906
US 1976-676505	19760413

ABSTRACT:
Polymethyl (unsatd. acyl) cyclohexenes and -cyclohexadienes and polymethylbicyclo[4.3.0]nona-2,8-dien-7-ones and -non-8-en-7-ones were prepd.; the first 2 types of ketones were useful in floral perfumes and all 4 ketone groups were useful as flavoring agents for foods and beverages (compns. given). Thus, 1-(1-hydroxy-3-butenyl)-2,6,6-trimethylcyclohexene was oxidized by Cr2O3 to 1-(3-butenoyl)-2,6,6-trimethylcyclohexene, and this was **isomerized** by p-MeC6H4SO3H in benzene to **trans**-1-crotonoyl-2,6,6-trimethylcyclohexene, which increased the power and richness of floral perfumes and was used in tutti-frutti flavoring compns., in flavor compns. for monastery type liquor, and in a soln. which increased the aromaticity of black tea.

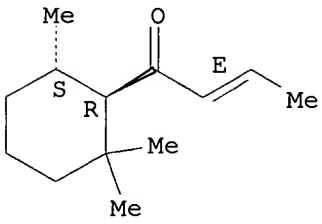
L5 ANSWER 18 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **58254-13-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and photolysis of)
RN 58254-13-0 CAPLUS
CN Ethanone, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1976:73332 CAPLUS
DOCUMENT NUMBER: 84:73332
TITLE: Photochemical reactions. 82. Photochemistry of .alpha.,.beta.-epoxy ketones. The .gamma.-hydrogen abstraction versus epoxy ketone rearrangement
AUTHOR(S): Mueller, Ernst Peter; Jeger, Oskar
CORPORATE SOURCE: Org.-Chem. Lab., ETH, Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1975), 58(7), 2173-88
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Photolysis of epoxyketone I(R = Me, R1 = H) gave **isomeric** epoxy alcohols II(R1 = H) and Me2C:CHCH2CH2COCH2Ac. Photolysis of I(R = R1 = Me) gave II(R1 = Me), whereas its 3,4-didehydro deriv. gave no isolable products. Similarly photolysis of I(R = R1 = H) gave no isolable products. The absence of **isomerization** of I to .beta.-diketones is attributed to steric factors.

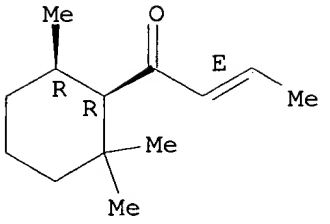
L5 ANSWER 19 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **52842-35-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(flavoring material and perfume, prepn. of)
RN 52842-35-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.beta.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



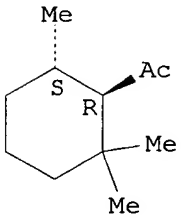
IT **52842-32-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(perfume, prepn. of)
RN 52842-32-7 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.alpha.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



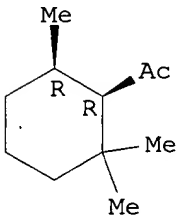
IT **52842-33-8P 52842-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation reaction with acetaldehyde)
RN 52842-33-8 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

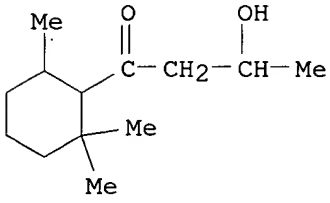


RN 52842-34-9 CAPLUS
CN Ethanone, 1-[(1R,6R)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

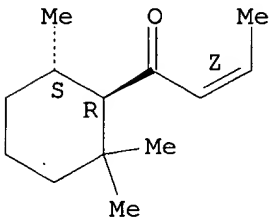


IT **39900-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydration of)
RN 39900-17-9 CAPLUS
CN 1-Butanone, 3-hydroxy-1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



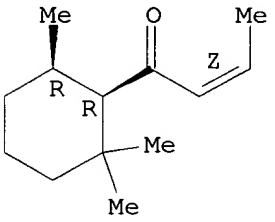
IT **52842-37-2P 56782-86-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 52842-37-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.beta.]-
(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 56782-86-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.alpha.]-
(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1975:478718 CAPLUS
DOCUMENT NUMBER: 83:78718
TITLE: Crotonoyltrimethylcyclohexane perfumes and flavoring materials
INVENTOR(S): De Haan, Douwe R.; Kettenes, Dirk K.
PATENT ASSIGNEE(S): Beheer, P. F. W., B. V., Neth.
SOURCE: Brit., 7 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1390654	A	19750416	GB 1972-49368	19731024
NL 7314428	A	19740501	NL 1973-14428	19731019
NL 177826	B	19850701		
NL 177826	C	19851202		
CA 1020582	A1	19771108	CA 1973-183974	19731023
BE 806536	A2	19740425	BE 1973-7000466	19731025
DE 2353578	A1	19740509	DE 1973-2353578	19731025
DE 2353578	C2	19850905		
AU 7361849	A1	19750501	AU 1973-61849	19731025
FR 2204625	A1	19740524	FR 1973-38245	19731026
JP 50052046	A2	19750509	JP 1973-120623	19731026

JP 57036252	B4	19820803			
IT 1003200	A	19760610	IT 1973-30634	19731026	
CH 585049	A	19770228	CH 1973-15092	19731026	
US 4109022	A	19780822	US 1976-681202	19760428	
US 4136066	A	19790123	US 1978-896224	19780413	
PRIORITY APPLN. INFO.:			GB 1972-49368	19721026	
			US 1973-409099	19731024	
			US 1976-681202	19760428	

ABSTRACT:

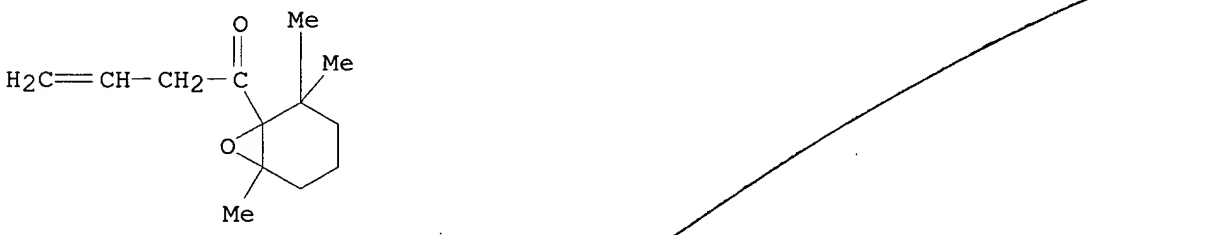
Trans,E-1-crotonoyl-2,2,6-trimethylcyclohexane (I), of a strong fresh fruity odor devoid of woody and .beta.-ionone character, was prepd. from ***cis*** -1-acetyl-2,2,6-trimethylcyclohexane by successive epimerization, condensation with MeCHO, and dehydration. I improved the flavor of raspberry and rhubarb flavoring compns. and of red currant juice conc. The **cis**,E- **isomer** (II), of a predominantly earthy-minty odor, was prepd. from ***cis*** -1-acetyl-2,2,6-trimethyl-4-cyclohexene by successive hydrogenation, condensation with MeCHO, and dehydration. The **trans**,Z-**isomer** (III) was prepd. from **trans**-dihydroionone by successive epoxidn., Wharton reaction, and oxidn. A 9:60:4:27 mixt. of I, II, III, and the ***cis*** ,Z-**isomer** was prepd. from .alpha.-ionone by successive epoxidn., hydrogenation, Wharton reaction, and oxidn.

L5 ANSWER 20 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

IT **31089-87-9P 31191-88-5P 35122-44-2P**
RL: PREP (Preparation)
(prepn. and use in perfume compns.)

RN 31089-87-9 CAPLUS

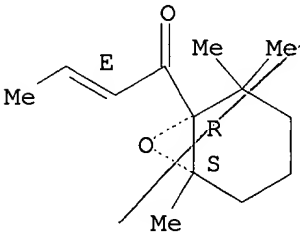
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



RN 31191-88-5 CAPLUS

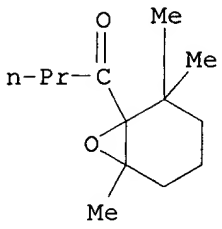
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 35122-44-2 CAPLUS

CN 1-Butanone, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



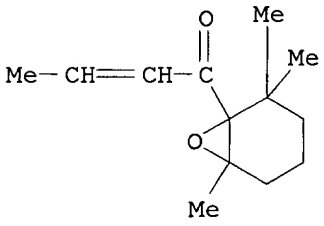
ACCESSION NUMBER: 1975:160116 CAPLUS
DOCUMENT NUMBER: 82:160116
TITLE: Use of alicyclic oxygenated compounds as perfume agents
INVENTOR(S): Schulte-Elte, Karl H.
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Patentschrift (Switz.), 9 pp. Division of Swiss 548,967 (CA 81: 77558t).
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 557422	A	19741231	CH 1972-16032	19710913

PRIORITY APPLN. INFO.: CH 1972-16032 19710913
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
I and II are prepd. and used in perfume compns. wherein R = CH(OH)CHn...CH...CH4-n (n = 1 or 2), CH(OH)Pr or COCH:CHCMe3, Y = CH(OAc)CHn...CH...CH4-n (n = 1 or 2), CH(OAc)Pr, COPr, and Z = pi bond or O. I were prepd. by the oxidn. of appropriate 1-cyclohexenes with singlet state O followed by treatment of the oxidn. product with a reducing agent. For example, a mixt. of 2,6,6-trimethyl-1-(1-hydroxy-2-butenyl)cyclohex-1-ene (III) [35124-05-1] (20.5 g), Rose Bengal (0.2 g), and NaOAc (1 g) in MeOH (160 ml) traversed by a stream of O was irradiated at 15.degree. with a Hg vapor lamp for 6 hr, and the resulting soln. (95 ml) was treated with a soln. of Na2SO3 (5 g) in 200 ml H2O first at 0-5.degree. and then at 40.degree. for 2 hr, and worked up to give by prep. gas chromatog. the following I (R = CH(OH)CH:CHMe, 2-substituent, **stereoisomer**, and % yield given): :CH2, threo, 30, (IV); :CH2, erythro, 6, (V); Me, -, 4 (VI). Also obtained was 48% ***trans*** -2,6,6-trimethyl-1-(2-butenoyl)-1,2-epoxycyclohexane [***31191-88-5***]. I with a 2-methylene group were also prepd. by treating appropriate epoxides with a basic agent. For example, a suspension of III (19.4 g) and NaOAc (12 g) in CH2Cl2 (35 ml) was treated with 40% aq. AcOOH (21 g) and NaOAc (0.6 g) at 20.degree. under a stream of N for 2 hr, and worked up to give the corresponding 1,2-epoxycyclohexane, (VII), b.0 4 84.degree.. VII (10.5 g) was treated with 50 ml of 1N soln. of Li in NH2CH2CH2NH2 and worked up to give in 22% yield a mixt. of IV and V. I (X = COCH:CHMe, 2-Me) was prepd. by oxidn. of VI with MnO2. CrO3/pyridine is an alternate oxidizing agent. II were prepd. from cyclohex-1-enes bearing appropriate hydroxyl-substituted Y groups by acetylation followed by epoxidation. For example, III was acetylated with AcCl/PhNMe2 to give II (Z = pi bond, Y = CH(OAc)CH:CHMe), (VIII), b.0 1 62.degree.. VIII was subjected to epoxidation and the product was sepd. by prep. gas chromatog. to give pure diastereoisomers of II (Z = O, Y = CH(OAc)CH:CHMe, threo 52%, erythro 47%). Perfume compns. incorporating the compds. were given.

L5 ANSWER 21 OF 35 CAPLUS

IT **51200-85-2P**
RL: PREP (Preparation)
(prepn. of)
RN 51200-85-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)

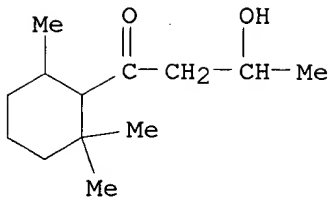


ACCESSION NUMBER: 1975:29926 CAPLUS
DOCUMENT NUMBER: 82:29926
TITLE: 2,6,6-Trimethyl-1-hydroxy-1-(2-butenoyl)-2-cyclohexene as a flavoring agent
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Patentschrift (Switz.), 3 pp. Division of Swiss 539,682 (CA 80;74276t).
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 551761	A	19740731	CH 1972-16847	19700414

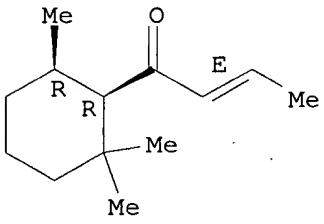
PRIORITY APPLN. INFO.: CH 1972-16847 19700414
ABSTRACT:
The title product (I) used at 0.1-10 ppm to give a honey-like aroma and flavor with a slight roasted hazelnut character was prepd. by adding 10 g of a mixt. of **cis**- and **trans**-2,6,6,-trimethyl-1-(2-butenoyl)-1,2-epoxycyclohexane to 2 g of acidified clay in 50 ml of dioxane, and heating to 100-5.degree. under N, termination of the reaction being detd. by gas chromatog., followed by washing, filtration, concn., and distn. at 80.degree./0.01 Torr, to give 8 g of the I, with n20 1.5049 and d20 1.018. I was used as a 1% EtOH soln. to flavor corn syrup at 0.03 g/100 ml.

L5 ANSWER 22 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **39900-17-9P 52842-32-7P 52842-33-8P**
52842-34-9P 52842-35-0P 52842-37-2P
52843-92-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 39900-17-9 CAPLUS
CN 1-Butanone, 3-hydroxy-1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



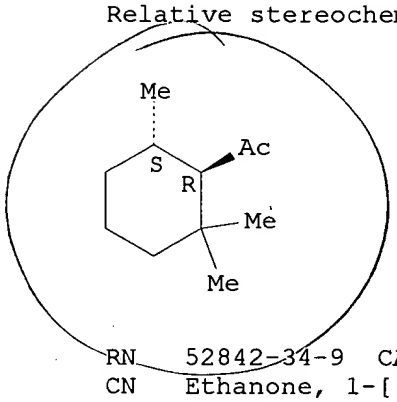
RN 52842-32-7 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.alpha.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



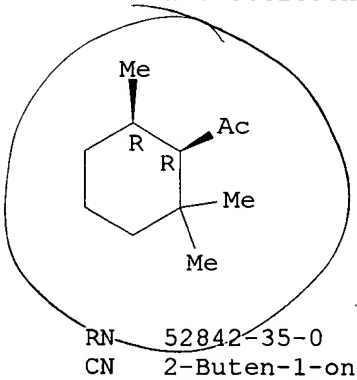
RN 52842-33-8 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



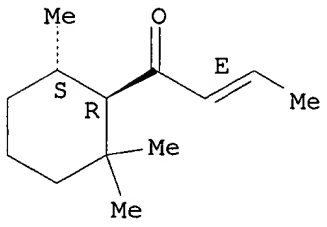
RN 52842-34-9 CAPLUS
CN Ethanone, 1-[(1R,6R)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



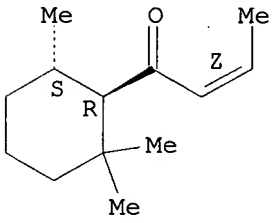
RN 52842-35-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.beta.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

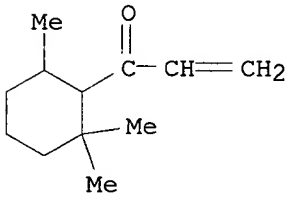


RN 52842-37-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.beta.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 52843-92-2 CAPLUS
CN 2-Propen-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.alpha.]-(9CI) (CA INDEX NAME)



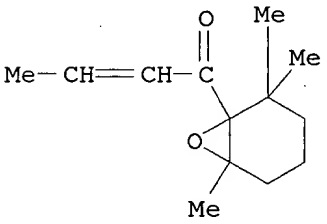
ACCESSION NUMBER: 1974:425196 CAPLUS
DOCUMENT NUMBER: 81:25196
TITLE: **Stereoisomers** of 1-crotonyl-2,2,6-trimethylcyclohexane for use in perfumes
INVENTOR(S): De Haan, Douwe R.; Kettenes, Dirk K.
PATENT ASSIGNEE(S): P.F.W. Beheer B. V.
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2353578	A1	19740509	DE 1973-2353578	19731025
DE 2353578	C2	19850905		
GB 1390654	A	19750416	GB 1972-49368	19731024

PRIORITY APPLN. INFO.: GB 1972-49368 19721026

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The four **stereoisomers** of 1-crotonyl-2,2,6-tri-methylcyclohexane (I, II, III, IV), useful as perfume ingredients, were prepd. by the epoxidn. of .alpha.-ionone, followed by hydrogenation over Pt to give a mixt. of epoxides, which, after reaction with N2H4 in AcOH and oxidn. with MnO2, gave a mixt. of I, II, III, and IV.

L5 ANSWER 23 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **51200-85-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acids)
RN 51200-85-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1974:74276 CAPLUS
DOCUMENT NUMBER: 80:74276
TITLE: Utilization of hydroxylated compounds as perfuming agents
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Patentschrift (Switz.), 3 pp. Division of Swiss 528,470 (Ger. 2,022,216, (CA 74;76564k).
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

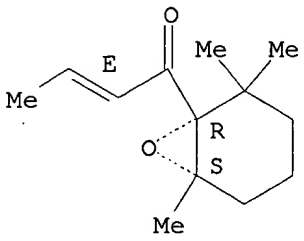
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 539682	A	19730914	CH 1972-12363	19700414

PRIORITY APPLN. INFO.: CH 1972-12363 19700414
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The title materials, such as 2,6,6-trimethyl-1-hydroxy-1-(2-butyryl)-2-cyclohexene (I), are prepd. and used at 0.1-1 wt.% of a perfume mixt. to improve the strength, diffusion, and richness of the perfume, and to give it a spicy note. I, b0.01 80.degree., is prepd. by treating **cis**- and ***trans*** -2,6,6-trimethyl-1-(2-butyryl)-1,2-epoxycyclohexane with an acid such as clayey earth, HCl, H3PO4, or H2SO4.

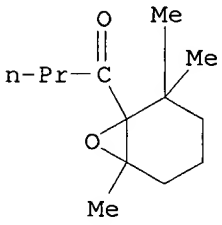
L5 ANSWER 24 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31191-88-5P 35122-44-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)-

(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 35122-44-2 CAPLUS
CN 1-Butanone, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



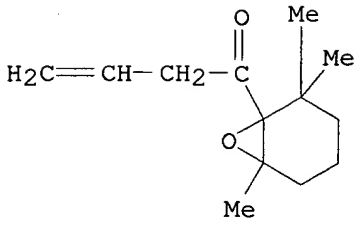
ACCESSION NUMBER: 1973:442041 CAPLUS
DOCUMENT NUMBER: 79:42041
TITLE: Oxygenated cycloaliphatics
INVENTOR(S): Schulte-Elte, Karl Heinrich
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 46 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2244680	A1	19730322	DE 1972-2244680	19720912
DE 2244680	C2	19821028		
CH 548967	A	19740515	CH 1971-13397	19710913

PRIORITY APPLN. INFO.: CH 1971-13397 19710913

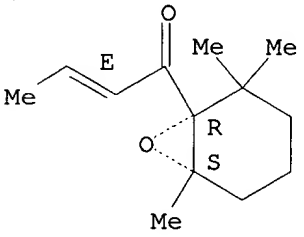
ABSTRACT:
The prepn. of a variety of cyclohexane derivs. (I-IV) with a fruity odor, useful as perfumes or in flavorings, was given. Thus, III (R = CHOHCH:CHMe) was oxidized by pure O, then reduced by Na2SO3 to give 48 **trans**-IV (R2 = COCH:CHMe), 30 threo- and 6 erythro-I [R2 = CH(OH)CH:CHMe, R1 = H], and 4% II (R and R1 same as in I).

L5 ANSWER 25 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31089-87-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**isomerization** of)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



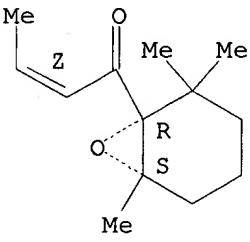
IT **31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)-
(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)-
(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1973:418207 CAPLUS
DOCUMENT NUMBER: 79:18207
TITLE: Cycloaliphatically unsaturated ketones
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 108 pp. Division of Ger. Offen. 2,022,216 (CA 74;76565k).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2065324	A1	19730329	DE 1970-2065324	19700506
DE 2065324	B2	19790726		
DE 2065324	C3	19800403		
CH 537452	A	19730713	CH 1969-12065	19690808
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
NL 7006649	A	19701110	NL 1970-6649	19700506
NL 163211	B	19800317		
NL 163211	C	19800815		
GB 1305621	A	19730207	GB 1970-22215	19700507
DD 96077	W	19730312	DD 1970-153631	19700507
JP 55003328	B4	19800124	JP 1970-38587	19700507
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

PRIORITY APPLN. INFO.:

CH 1969-6976	19690507
CH 1969-12065	19690808
CH 1970-5559	19700414
CH 1970-5725	19700417
CH 1967-15667	19671109
CH 1968-16309	19681101
US 1968-774179	19681107
CH 1970-6725	19700417
US 1970-35594	19700507
US 1974-503738	19740906
US 1976-676505	19760413

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:
MeCH:CMeCH2CHMeCH:CMeCHO was cyclized to 2,4,6,6-tetramethyl-1-cyclohexene-1-carboxaldehyde, which was treated with MeCH:CH2Li to give an alc., which was oxidized to the ketone I. Approx. 20 other ethylenic cyclohexyl ketones were prepd. similarly; these compds. had a pleasant odor, usually fruity, and formulations were given for their use in perfumes and as flavoring materials for liqueurs and foods.

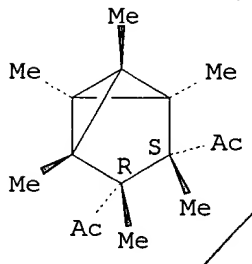
L5 ANSWER 26 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

IT **41049-45-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 41049-45-0 CAPLUS

CN Ethanone, 1,1'-(1,2,3,4,5,6-hexamethyltricyclo[3.1.0.02,6]hexane-3,4-diyl)bis-, stereoisomer (9CI) (CA INDEX NAME)

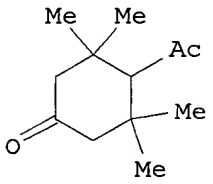
Relative stereochemistry.



ACCESSION NUMBER: 1973:135392 CAPLUS
DOCUMENT NUMBER: 78:135392
TITLE: Small rings. 13. Direct cyclobutene-bicyclobutan valence **isomerization**

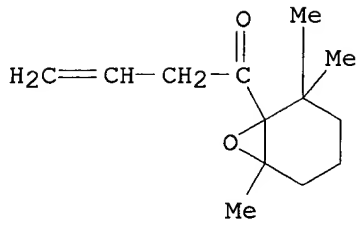
AUTHOR(S): Maier, Guenther; Schneider, Manfred
CORPORATE SOURCE: Fachberich Chem., Univ. Marburg, Marburg/L., Fed. Rep. Ger.
SOURCE: Angewandte Chemie (1973), 85(4), 174-5
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The ozonide (i) and Ag Bf4 16 hr at 20.degree. in Me2CO under N, gave 90.degree. ozonide (ii) by cyclobutene-bicyclobutane **isomerization**. The stereochem. of the **isomerization** was discussed.

L5 ANSWER 27 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **16556-46-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16556-46-0 CAPLUS
CN Cyclohexanone, 4-acetyl-3,3,5,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



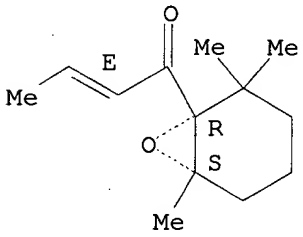
ACCESSION NUMBER: 1972:139997 CAPLUS
DOCUMENT NUMBER: 76:139997
TITLE: Synthesis of 3,3,5,5-4-acetyl-1-cyclohexanone
AUTHOR(S): Heymes, A.; Teisseire, P.
CORPORATE SOURCE: Cent. Rech., Roure Bertrand Files et J. Dupont, Grasse, Fr.
SOURCE: Recherches (1971), No. 18, 104-8
CODEN: RCHEAC; ISSN: 0557-6970
DOCUMENT TYPE: Journal
LANGUAGE: French
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The title compd. (I) was prepd. by addn. of MeMgI-FeCl3 to isophorone, decompn. of the product on ice to yield 3,5,5-trimethyl-3-cyclohexen-1-one (II), oxidn. of II in Et2O with o-HO2CC6H4CO2OH and treatment with 10% NaOH to give 3,5,5-trimethyl-4-hydroxy-2-cyclohexen-1-one, **isomerization** of the product in C6H6 with p-MeC6H4SO3H to yield 3,5,5-trimethyl-1,4-cyclohexanedione, ketalization of the dione to the monoethylene ketal (III), reaction of III and NaC.tplbond.CH in liq. NH3 to give 62% 1-ethynyl-2,6,6-trimethyl-4-(ethylenedioxy-1-cyclohexanol, decompn. of the alc. in refluxing HCO2H to 3,5,5-trimethyl-4-acetyl-2-cyclohexen-1-one (IV), and addn. of LiMe2Cu to IV to give 60% I.

L5 ANSWER 28 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31089-87-9P 31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



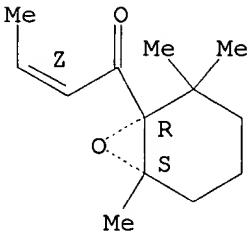
RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)-
(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)-
(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1971:76564 CAPLUS
DOCUMENT NUMBER: 74:76564
TITLE: Cycloaliphatic unsaturated ketones for use as perfumes
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Stoll, Max; Ohloff, Guenther
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 137 pp. Addn. to Ger. Offen. 1,807,568
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2022216	A	19701119	DE 1970-2022216	19700506
DE 2022216	B2	19760701		
DE 2022216	C3	19770217		
CH 537452	A	19730713	CH 1969-12065	19690808

CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
NL 7006649	A	19701110	NL 1970-6649	19700506
NL 163211	B	19800317		
NL 163211	C	19800815		
GB 1305621	A	19730207	GB 1970-22215	19700507
DD 96077	W	19730312	DD 1970-153631	19700507
JP 55003328	B4	19800124	JP 1970-38587	19700507
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

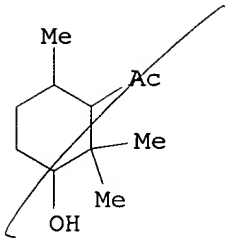
PRIORITY APPLN. INFO.:

CH 1969-6976 19690507
CH 1969-12065 19690808
CH 1970-5559 19700414
CH 1970-5725 19700417
CH 1967-15667 19671109
CH 1968-16309 19681101
US 1968-774179 19681107
CH 1970-6725 19700417
US 1970-35594 19700507
US 1974-503738 19740906
US 1976-676505 19760413

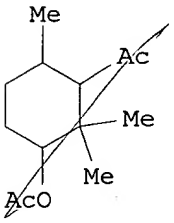
ABSTRACT:

Stereoisomers of cyclic unsatd. ketones (I-V, R, R1, R2, R3 = H or Me) were prepd. A mixt. of MeCH:CMeCH2CHMeCH:CMeCHO and MeCH:CMeCH2CMe2CH:CHCHO was treated with PhNH2-Na2SO4 in Et2O to give a 4-methyl-.alpha. and 4-methyl-.beta.-cyclocitral mixt., which was treated with alc. KOH to give 4-methyl-.beta.-cyclocitral (VI). VI was treated with MeCH:CHLi to give 2,4,6,6-tetramethyl-1-(1-hydroxy-2-butenyl)-1-cyclohexene, which was oxidized with MnO2 to give 2,4,6,6-tetramethyl-1-**trans**-crotonoyl-1-cyclohexene (I, R = R1 = R3 = H, R2 = Me) (VII). Dehydrogenation of VII with N-bromosuccinimide-azodiisobutyronitrile in CH2Cl2 gave 2,4,6,6-tetramethyl-1-**trans**-crotonoyl-1,3-hexadiene (II, R = R1 = R3 = H, R2 = Me): .apprx.11 I-II were also prepd. 2,6,6-Trimethyl-1-(1-hydroxy-3-butenyl)-1-cyclohexene was epoxidized with Ac-O2H-NaOAc to give 2,6,6-trimethyl-1-(1-hydroxy-3-butenyl)-1,2-epoxycyclohexane, which was oxidized with Na2Cr2O7 (to give the corresponding ketone), followed by treatment with NaOAc in dioxane, to give **cis**- and **trans**-2,6,6-trimethyl-1-crotonoyl-1,2-epoxycyclohexane (III, R = R1 = R2 = R3 = H). Treatment of the **cis**-**trans**-epoxycyclohexane mixt. with acidc kieselguhr in dioxane gave 2,6,6-trimethyl-1-hydroxy-1-crotonyl-2-cyclohexane. Cyclization of 2,6,6-trimethyl-1-(2-methylcrotonoyl)-1-cyclohexene (I, R = R2 = R3 = H, R1 = Me) with acidic kieselguhr in dioxane gave 1,5,5,8,9-pentamethylbicyclo-[4.3.0] non-8-en-7-one (IV, R = H, R1 = Me). Cyclization of 2,6,6-trimethyl-1-crotonoyl-2-cyclohexene in the presence of BF3 in benzene gave 4,4,8-trimethyl-9-methylenebicyclo [3.3.1]-non-6-ene (V).

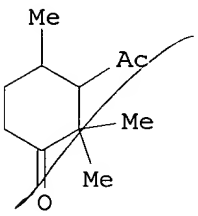
L5 ANSWER 29 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **27243-02-3P 27243-03-4P 27243-04-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 27243-02-3 CAPLUS
CN Ketone, 3-hydroxy-2,2,6-trimethylcyclohexyl methyl (8CI) (CA INDEX NAME)



RN 27243-03-4 CAPLUS
CN Ketone, 3-hydroxy-2,2,6-trimethylcyclohexyl methyl, acetate (8CI) (CA INDEX NAME)



RN 27243-04-5 CAPLUS
CN Cyclohexanone, 3-acetyl-2,2,4-trimethyl- (8CI) (CA INDEX NAME)

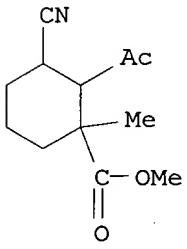


ACCESSION NUMBER: 1970:121720 CAPLUS
DOCUMENT NUMBER: 72:121720
TITLE: Synthesis of alicyclic compounds
AUTHOR(S): Aguilar, Carlos; Salmon, Manuel; Walls, Fernando
CORPORATE SOURCE: Inst. Quim., Mexico, D. F., Mex.
SOURCE: Boletin del Instituto de Quimica de la Universidad Nacional Autonoma de Mexico (1969), 21, 226-40
CODEN: BIQUA5; ISSN: 0076-745X
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
ABSTRACT:

A soln. of 152 g citral in 320 ml Et2O was added to a Grignard reagent, prepd. from 24.3 g Mg and 141.9 g MeI in 310 ml Et2O. Decompn. of the complex with H2O gave 89.2% of a mixt. of **cis**- and **trans** -.alpha.-methylgeraniol (**trans**-I); oxidn. of 20 g of this mixt. with 200 g active MnO2 in 900 ml hexane gave 14 g of a mixt. of **cis**-and ***trans*** -4,8-dimethyl-3,7-nonadien-2-one (**trans**-II), (35:65%, resp.) b10 95.degree.. The **isomers** were sepd. by TLC; **cis** ***isomer*** b1 80.degree., **trans isomer** b2 75.degree.. The **cis isomer** equilibrated rapidly to the 35:65 mixt. Treating 5 g I with 5 ml 5% H2SO4 and 5 ml AcOH, stirring the mixt. 17 hr at room temp., gave, upon chromatog. (SiO2, C6H6 eluent) an unid entified first fraction and 1.1 g 1,3-dimethyl-4-(1-methyl-1-hydroxyethyl) -1-cyclohexene

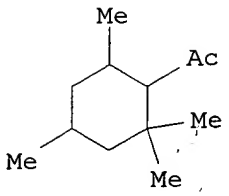
(III), b2 75.degree.. To 5 g II, 23 ml 75% H_2SO_4 was added with cooling, the mixt. stirred 4 hr, and worked up by TLC, isolating 3 fractions: the first was not investigated, the 2nd one was identified as II, and the most polar fraction further purified by chromatog. over SiO_2 gave 125 mg 2,2,4-trimethyl-3-acetyl-1-cyclohexanol (IV), b1 65.degree.. Oxidn. of 150 mg IV in 7 ml anhyd. Me_2CO with Jones reagent and purification of the reaction product by TLC, gave 140 mg 2,2,4-trimethyl-3-acetyl-1-cyclohexanone, m. 52.degree.. A mixt. of 3.0 g II (mixed **isomers**) and 10 ml 98% HCO_2H was stirred 48 hr and worked up by chromatog. (SiO_2, 50:50 C_6H_6-AcOEt eluent) and final TLC, to give 0.510 g V , b1 155.degree.. Ir, NMR, and mass spectra of the compds. were shown.

L5 ANSWER 30 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **23477-94-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 23477-94-3 CAPLUS
CN Cyclohexanecarboxylic acid, 2-acetyl-3-cyano-1-methyl-, methyl ester, stereoisomer (8CI) (CA INDEX NAME)



ACCESSION NUMBER: 1969:470168 CAPLUS
DOCUMENT NUMBER: 71:70168
TITLE: Synthesis of **racemic cis, trans**-1,3-dimethylcyclohexane-1,2,3-tricarboxylic acid-a degradation product of agathic acid
AUTHOR(S): Banerjee, Dilip Kumar; Ranganathan, R.
CORPORATE SOURCE: Indian Inst. Sci., Bangalore, India
SOURCE: Bulletin of the National Institute of Sciences of India (1968), No. 37, 125-36
CODEN: BNSIAE; ISSN: 0027-9528
DOCUMENT TYPE: Journal
LANGUAGE: English
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
A synthesis of **cis,trans**-1,3-dimethylcyclohexane-1,2,3-tricarboxylic acid, (I) a degradation product of agathic acid, is described. Stereochem. assignments were made by a study of the N.M.R. spectra of crucial intermediates. Chem. confirmation of these assignments was also provided.

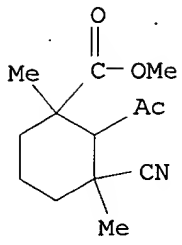
L5 ANSWER 31 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **3212-56-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 3212-56-4 CAPLUS
CN Ketone, methyl 2,2,4,6-tetramethylcyclohexyl (6CI, 7CI, 8CI) (CA INDEX NAME)



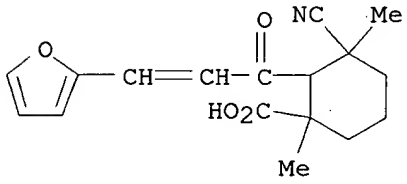
Maybe

ACCESSION NUMBER: 1967:38055 CAPLUS
DOCUMENT NUMBER: 66:38055
TITLE: Syntheses of terpenes by the condensation of aliphatic compounds. II. Self-condensation of mesityl oxide and structures of **isomeric** isoxylitones
AUTHOR(S): Ueda, Hiroo; Takeo, Kenichi; Tsai, Ping-Li; Tatsumi, Chuji
CORPORATE SOURCE: Univ. Osaka Prefect., Sakai, Japan
SOURCE: Agricultural and Biological Chemistry (1966), 30(10), 1004-14
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
cf. CA 64, 15927e. NaOBu-tert (13 g. Na and 100 ml. tert-BuOH) in 300 ml. C6H6 was added at 15.degree. to 98 g. mesityl oxide in 400 ml. C6H6 in 30 min. The mixt. was stirred 4 hrs. at 15.degree., washed with water, dried, and distd. at 82-9.degree./3 mm. Gas chromatography of the product yielded isoxylitone-A (dinitrophenylhydrazone m. 176-7.degree.; semicarbazone m. 178-9.degree.) (I), isoxylitone-B (dinitrophenylhydrazone m. 156-7.degree.; semicarbazone m. 177-78.degree.) (II), isoxyletone-C (dinitrophenylhydrazone m. 102-4.degree.) (III), isoxylitone-D (dinitrophenylhydrazone m. 131-2.degree.; semicarbazone m. 166-7.degree.) (IV), and isophorone). The structures of I and II were given as conformers of 1-acetyl-2,4,6,6-tetramethyl-1,3-cyclohexadiene, sepd. by the rotational barrier of an acetyl group and interconversional barrier of a cyclohexadiene ring. III and IV were 4-isopropenyl-1,5,5-trimethyl-1-cyclohexen-3-one and 5,5-dimethyl-3-(1-isobuteneyl)-2-2cyclohexen-1-one, resp. Catalytic redn. of I and II gave tetrahydroisoxylitone, b4 77.3-78.0.degree. (V) (dinitrophenylhydrazone m. 88.5-9.0.degree.; semicarbazone m. 167.5-8.0.degree.). I and II interconverted by refluxing in 20% H2SO4. Oxidn. of II with NaMnO4 yielded CO2, AcOH, and a compd., esterfication of which gave Et mesitonate. Oxidn. of V with KOBr gave an oil, b3 104-7.degree., which was brominated to 1-bromo-2,4,6,6,-tetramethylcyclohexane, b8.5 82.5-3.0.degree.. The latter was refluxed with collidine to give 2,4,6,6-tetramethyl-1-cyclohexane, b 150.degree., which was ozonized and esterified to give Et 6-oxo-2,2,4-trimethylheptanoate.

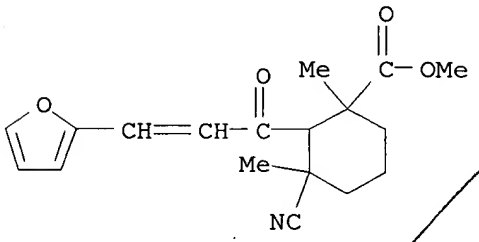
L5 ANSWER 32 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **10207-52-0**, Cyclohexanecarboxylic acid, 2-acetyl-3-cyano-1,3-dimethyl-, methyl ester **10207-55-3**, Cyclohexanecarboxylic acid, 3-cyano-2-[3-(2-furyl)acryloyl]-1,3-dimethyl- **10207-56-4**, Cyclohexanecarboxylic acid, 3-cyano-2-[3-(2-furyl)acryloyl]-1,3-dimethyl-, methyl ester **10207-91-7**, Cyclohexanecarboxylic acid, 2-acetyl-3-cyano-1-methyl-, methyl ester
(prepn. of)
RN 10207-52-0 CAPLUS
CN Cyclohexanecarboxylic acid, 2-acetyl-3-cyano-1,3-dimethyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)



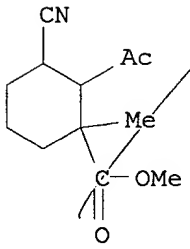
RN 10207-55-3 CAPLUS
CN Cyclohexanecarboxylic acid, 3-cyano-2-[3-(2-furyl)acryloyl]-1,3-dimethyl- (7CI, 8CI) (CA INDEX NAME)



RN 10207-56-4 CAPLUS
CN Cyclohexanecarboxylic acid, 3-cyano-2-[3-(2-furyl)acryloyl]-1,3-dimethyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)



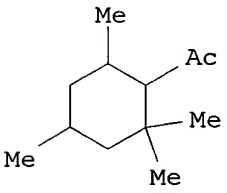
RN 10207-91-7 CAPLUS
CN Cyclohexanecarboxylic acid, 2-acetyl-3-cyano-1-methyl-, methyl ester (7CI, 8CI) (CA INDEX NAME)



ACCESSION NUMBER:	1966:473708 CAPLUS
DOCUMENT NUMBER:	65:73708
ORIGINAL REFERENCE NO.:	65:13772f-h
TITLE:	Syntheses of the **trans**, meso, and **racemic** C11 acids, degradation products of diterpene-acids
AUTHOR(S):	Banerjee, D. K.; Balasubrahmanyam, S. N.; Ranganathan, R.

CORPORATE SOURCE: Indian Inst. Sci., Bangalore
SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (16), 1458-67
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
Syntheses of the **isomers** of the title C11 acid, 1(a),-3(a)-dimethylcyclohexane-1(e),2(e),3(e)-tricarboxylic acid (I) and 1-(a),3(e)-dimethylcyclohexane-1(e),2(e),3(a)-tricarboxylic acid (II), the latter by 2 different routes, are reported. Two of the 4 possible ***isomers*** of the precursor triester, trimethyl 1-methyl cyclohexane-1,2,3,-tricarboxylate, on individual methylation followed by hydrolysis, gave **trans**,meso-I, identified by comparison with an authentic sample, and **cis,trans**-(II) whose structure and configuration were proved by comparison with a specimen obtained by the unambiguous and highly stereoseleetive 2nd synthesis. This demonstrated that methylation of the triester **isomers** occurs stereospecifieally and exclusively at C-3. In the 2nd sequence, it has been possible to assign definite conformations to 4 key intermediates and the final product, directly from N.M.R. spectra, from changes in these spectra accompanying specific steps, and from chem. evidence. Comparison of the N.M.R. spectra of the ***isomeric*** triesters of I and II has provided unequivocal proof of the accepted **trans**,meso configuration for the abietic acid degradation product I. a and e are axial and equa-torial, resp. 30 references.

L5 ANSWER 33 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **3212-56-4**, Ketone, methyl 2,2,4,6-tetramethylcyclohexyl (prepn. of)
RN 3212-56-4 CAPLUS
CN Ketone, methyl 2,2,4,6-tetramethylcyclohexyl (6CI, 7CI, 8CI) (CA INDEX NAME)

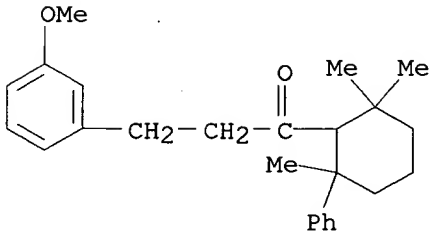


ACCESSION NUMBER: 1965:462535 CAPLUS
DOCUMENT NUMBER: 63:62535
ORIGINAL REFERENCE NO.: 63:11379b-h,11380a
TITLE: Condensation of mesityl oxide in alkaline medium. Structure of isoxylitones
AUTHOR(S): Furth, Bernard; Wiemann, Joseph
CORPORATE SOURCE: Lab. Chim. Org. Struct., Paris
SOURCE: Bulletin de la Societe Chimique de France (1965), (6), 1819-31
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Self-condensation of the title compd. (I) in the presence of a variety of catalysts does not influence the nature of the **isomeric** C12H18O products. The ratio of these products to one another and the overall yield of C12H18O **isomers** is affected by the choice of catalyst. Vapor phase chromatography on a column impregnated with 20% silicone oil at 200.degree.

divided the **isomeric** product into 4 peaks, corresponding to isophorone (II), component AIX (III), C12 isoxylitones (IV), and compd. BIX (V). On a polar column of cyanosilicone at 200.degree., III gave seven peaks, one of which was II; IV sepd. into five **isomers**; and V gave a single peak. Heterogeneous catalysis with MgO gave a product giving all the mentioned peaks on chromatography in appreciable amounts; BaO gave better yields, with less III and more V and higher products. CaO was only slightly active, but IV was detected in the product. NaNH2 gave a rapid reaction with a product containing almost equal amts. of dimerized products as higher products. Allassion and Dowex basic exchange resins gave similar mixts. of ***isomers*** as the other catalysts, with a predominance of IVa and IVb. ZnO and Al2O3 gave extremely complex mixts. of products; at high temps., I degraded to give CO2 and lacrimatory, acidic products. Homogeneous catalysis with Na tert-amylate gave a product with little III and higher products and a predominance of IVa and IVb. NaOEt gave similar results, except that there were more higher products. PhCH2Me3NOH gave increased quantities of IVb, IVc, and IVd, but little III and V. Treatment of I with NaOH or KOH in MeOH gave Me2CO, II, and a higher percentage of polymers; the results were not very reproducible. Treatment of IV with NaOBr showed that IVa and IVb bore an Ac group. Hydrogenation of IVa and IVb gave 1-(2-acetonyl)-3,3,5-trimethylcyclohexane, Wolfe-Kishner-Minlon redn. of which gave 1-propyl-3,3,5-trimethylcyclohexane (VI). Treatment of isophorone with propylmagnesium bromide followed by redn. over Raney Ni gave two ***isomers*** identical to the two **isomers** of VI obtained from IVa and IVb. From this evidence and the comparison of IVa and IVb to the isoxylirones in which the C:O group is **cis** and **trans** to the closest C:C bond by N.M.R. spectroscopy, it was shown that IVa and IVb are ***cis*** and **trans** forms of the same compd. IVc, IVd, and IVe had no Ac group and it is suggested, on the basis of uv and ir evidence that they arise from an .alpha.-Michael addn. III was shown to contain 35% of a compd. having an Ac group by N.M.R. spectroscopy. Ir spectra indicated conjugated and non-conjugated C:O groups, and three C:C bonds. From the mixt., two 2,4-dinitrophenylhydrazone (DNP) derivs., m. 85.degree. and m. 160.degree., were isolated. Hydrogenation gave a mixt. resolvable into 4 peaks on vapor-phase chromatography. One of these corresponded to tetrahydroisoxylitone. It is suggested that one of the components of III is a non-conjugated ethylenic ketone with the same C skeleton as IVa and IVb, and of the non-acetylated products, one at least is a conjugated ketone. V, by comparison with the vapor-phase chromatography retention time and ir of the genuine compd., was shown to be 3-(2-methyl-2-propenyl)-5,5-dimethyl-1-2-cyclohexenone. V gives a semicarbazone, m. 167.degree., and takes up 2 moles H on Pd-C to give the corresponding satd. ketone, b12 124.degree.; DNP, m. 111.degree.. It is suggested that V arises by an .alpha.-Michael addn. followed by a crotonization reaction. In certain of the condensations, a ketol (VII), b12 100-15.degree., was obtained. VII was also obtained when I was dimerized in the presence of Li. The structure was shown by N.M.R. spectroscopy. Basic dehydration of VII showed it to be an intermediate in the formation of the I dimers; dehydration with p-MeC6H4SO3H or iodine gave 1-acetyl-2,2,4-trimethyl-6-methylene-4-cyclohexene. Addn. of K in alcohol to this compd. converts it to IVa and IVb; hydrogenation on Pd-C gives 1-acetyl-2,2,4,6-tetramethylcyclohexane, b12 94-6.degree.. It is suggested that in the dimerization of I, VII is formed by a .gamma.-Michael addn. IVa and IVb can be obtained from this by a retroketolization with ring-opening. Pivoting around the C-4-C-5 bond makes possible a crotonization leading to IVa and IVb.

L5 ANSWER 34 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
IT **114280-31-8**, 1-Propanone, 3-(m-methoxyphenyl)-1-(2,2,6-trimethyl-6-phenylcyclohexyl)-
(prepn. of)
RN 114280-31-8 CAPLUS
CN 1-Propanone, 3-(m-methoxyphenyl)-1-(2,2,6-trimethyl-6-phenylcyclohexyl)-

(6CI) (CA INDEX NAME)



ACCESSION NUMBER: 1959:17417 CAPLUS
DOCUMENT NUMBER: 53:17417
ORIGINAL REFERENCE NO.: 53:3269c-i,3270a-e
TITLE: Experiments on the synthesis of diterpenes. I. A total synthesis of (.+-.)-totarol
AUTHOR(S): Barltrop, J. A.; Rogers, N. A. J.
CORPORATE SOURCE: Univ. Oxford, UK
SOURCE: Journal of the Chemical Society, Abstracts (1958) 2566-72
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ABSTRACT:

Refluxing 3.42 g. 2-acetyl-1,3,3-trimethylcyclohexene, 2.72 g. m-MeOC6H4CHO, and 0.56 g. KOH in 30 ml. EtOH 30 min., adding AcOH until acid, and working up gave 3.49 g. 2-(.beta.-m-methoxyphenylacryloyl)-1,3,3-trimethylcyclohexene (I), b0.1 166-9.degree.. I (3.25 g.) in 40 ml. EtOH and 1.1 moles H under atm. pressure over Raney Ni gave 2.75 g. 2-(.beta.-m-methoxyphenylpropionyl)-1,3,3-trimethylcyclohexene (II), b0.1 185-90.degree.. II (5.72 g.) in PhNO2 satd. with HCl and AlCl3 stirred 20 hrs. at room temp. gave 1.01 g. 5-methoxyindan-1-one (III), b0.2 145-50.degree., m. 108.degree.; semicarbazone, m. 237.8.degree.. Stirring 5.01 g. II with 50 ml. 90% H3PO4, 5 hrs. at 140-50.degree. under N gave 2.01 g. III. Treating 10 g. I in 120 ml. C6H6 with 18 g. AlCl3 in 100 ml. C6H6, passing HCl through the soln. during the 1 hr. of addn. and then 1 hr. longer, stirring 2 hrs., and pouring the mixt. on 2N HCl and ice, extg. with Et2O and distg. gave 0.2 g. 1,3,3-trimethyl-1-phenylcyclohexane, b0.2 78-83.degree., 3.3 g. I, and 2.2 g. 2-(.beta.-m-methoxyphenylpropionyl)-1,3,3-trimethyl-1-phenylcyclohexane, b0.2 195-200.degree.. Adding 3.4 g. 2,2,6-trimethylcyclohexanone in 30 ml. anhyd. Et2O dropwise to a mixt. of 2.44 g. PhC.tplbond.CH, 30 ml. Et2O, KNH2 (from 1 g. K) in 100 ml. liquid NH3, stirring for 2 hrs., then adding H2O, extg. with Et2O, and distg. gave 2.47 g. 2,2,6-trimethyl-1-phenylethynylcyclohexanol (IV), b0.15 153-6.degree.. IV (2.45 g.) in 70 ml. AcOEt and H over 5% Pd-C at 1 atm. and room temp. gave 2.4 g. 2,6,6-trimethyl-1-phenylcyclohexanol (V), b0.1 172-7.degree.. Stirring 2.3 g. V with 20 ml. 90% H3PO4 and 25 g. P2O5 under N 45 min. at 95.degree., the mixt. cooled and added to 200 ml. H2O and extd. with Et2O, the ext. washed with brine, dried, and distd. gave 1.6 g. 1,2,3,4,9,10,11,12-octahydro-1,1,12-trimethylphenanthrene, b0.05 108-10.degree.. Adding 9.8 g. 2,2,6-trimethylcyclohexanone in 90 ml. Et2O dropwise with stirring to 9.8 g. m-MeOC6H4C.tplbond.CH in 90 ml. Et2O, and KNH2 (3.75 g. K) in 450 ml. liquid NH3 and stirring 1 hr. more gave 15.75 g. 1-(m-methoxyphenylethynyl)-2,2,6-trimethylcyclohexanol (VI), b0.1 180-5.degree.. Hydrogenation of 15.7 g. VI, as above, gave 15.5 g. 1-(m-methoxyphenethyl)-2,2,6-trimethylcyclohexanol (VII), b0.15 210-15.degree.. Stirring 10 g. VII under N with 120 ml. sirupy H3PO4 and 150 g. H3PO4 45 min. at 85.degree. gave 7.93 g. **trans**-1,2,3,4,9,10,11,12-octahydro-7-methoxy-1,1,12-trimethylphenanthrene (VIII), b0.1 155-60.degree., m. 52-5.degree.. Treating 7.93 g. VIII in 400 ml. Et2O and 1 l. liquid NH3 with 3.5 g. Li in small pieces with stirring, stirring 10 min., then 50 ml. EtOH added dropwise over 20 min., 500 ml. H2O added after the reaction stopped and

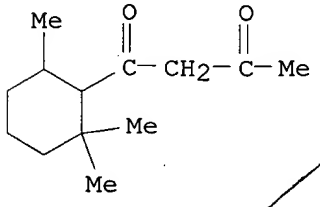
NH3 evapd., and the soln. extd. with Et2O to give 7.02 g. oil (IX). Heating 3.5 g. IX, 150 ml. EtOH, and 120 ml. 5N HCl 30 min. at 60.degree., then pouring into ice water and working up gave 2.7 g. of a pale yellow oil which, on chromatographing on alumina and eluting with light petroleum, yielded 720 mg. unchanged VIII; further elution with 10% C6H6 in light petroleum gave 780 mg. podocarp-13(14)- and 897 mg. podocarp-8(14)-en-7-one (X), m. 89-90.degree.; semicarbazone, m. 213-15.degree. (decompn.). Treating 3.5 g. IX with 7.5 g. oxalic acid and 10 ml. H2O 40 min. at 25.degree., adding the mixt. to 500 ml. H2O, and working up gave an oil which, on chromatographing on alumina and eluting with ligroine yielded 700 mg. unchanged VIII; further elution with 10% C6H6 in ligroine gave 2.65 g. podocarp-13(14)-en-7-one (XI), m. 101-3.degree.. Heating 530 mg. XI with 20 ml. EtOH and 15 ml. 5N HCl 30 min. at 90.degree., working up as above and chromatographing gave 170 mg. unchanged XI and 195 mg. X. The infrared spectra of (+)- and (.+-.)-X semicarbazone in Nujol were identical apart from slight differences. Refluxing 16.1 mg. (+)-X semicarbazone with 5 ml. 2N HCl and 1 ml. EtOH 20 min., adding H2O, and extg. the mixt. with Et2O, gave 11.7 mg. oil, which [showing, by its infrared spectra, some **isomerization** to the 13(14)-**isomer**] was chromatographed and eluted with 1:1 C6H6-ligroine to give 2.0 mg. (+)-X. Treating 415 mg. X in 8 ml. iso-PrBr with M tert-AmONa in 15 ml. C6H6 under N, refluxing 3.5 hrs., cooling, shaking with 25 ml. 2N HCl, and isolating with Et2O, gave 175 mg. yellow oil, b0.5 155-60.degree., whose infrared spectra indicated the presence of both totar-8(14)- and totar-13(14)-en-7-one. Similar treatment of 760 mg. mixt. of X and XI gave 267 mg. 8-isopropyltotar-13(14)-en-7-one, b0.1 165-70.degree., on elution with ligroine; further elution with 1:1 C6H6-ligroine gave 202 mg. mixt. of totaren-7-ones. Similar treatment of 680 mg. XI gave 690 mg. yellow oil which, on distn., gave a mixt. of totaren-7-ones. The synthetic mixt. of totaren-7-ones (420 mg.) and 290 mg. N-bromosuccinimide refluxed in CCl4 30 min., the mixt. cooled, filtered, washed with 10% Na2CO3, and evapd. gave a pale yellow viscous oil which on heating to 100.degree. under vacuum lost some HBr, leaving 400 mg. residue; this was refluxed with .gamma.-collidine 2.5 hrs., the .gamma.-collidine vacuum distd., 15 ml. 5N HCl added, and the product (XII) isolated with Et2O; XII was a clear brown glass (380 mg.), whose infrared spectra showed bands for (.+-.)-totarol, a weak band at 5.85 .mu., and a moderately intense band at 6.0.mu.; the residue was chromatographed and eluted with ligroine to give 118 mg. of a ketone; further elution with 1:1 C6H6-ligroine gave 182 mg. of a pale yellow glass; the fractions contg. least ketonics (83 mg.) were rechromatographed and eluted with 1:1 C6H6-ligroine to give 15.8 g. of totaren-7-ones; further elution with C6H6 gave 35.3 mg. (.+-.)-totarol, b0.2 170-5.degree.. (.+-.)-Totaryl benzoate was a glass, b. 145-50.degree./2 .times. 10-5 mm.

L5 ANSWER 35 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

IT **39900-14-6**, 1,3-Butanedione, 1-(2,2,6-trimethylcyclohexyl)-
(prepn. of)

RN 39900-14-6 CAPLUS

CN 1,3-Butanedione, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1949:25971 CAPLUS

DOCUMENT NUMBER: 43:25971

ORIGINAL REFERENCE NO.: 43:4813c-i,4814a

TITLE: Violet perfumes. XXVIII. Ketotetrahydroionone

AUTHOR(S): Prelog, V.; Frick, H.
SOURCE: Helvetica Chimica Acta (1948), 31, 2135-42
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
ABSTRACT:
cf. C.A. 43, 3798d. In an unsuccessful effort to determine the structure of the tetrahydroionone deriv. (I), contg. an addnl. O function, which was isolated from pregnant mare's urine (C.A. 43, 3798f), .alpha.'-, .beta.'-, and 4-ketotetrahydroionones were prepd. **cis**-Tetrahydroionone (1.0 g.) in 4 cc. abs. alc. with 4 drops concd. H_2SO_4 was decompd. at 45.degree. with 1.1 g. n-$BuNO_2$ heated 2 hrs. at 45.degree., taken up in Et_2O, extd. with 10% NaOH, and the alk. ext. acidified to give 0.45 g. of the .alpha.'-iso-nitroso deriv.; steam distn. from 4 g. $(COOH)_2$ gave 0.25 g. .alpha.'-keto-**cis**-tetrahydroionone, b0.1 100-20.degree. [bis-(phenylsemicarbazone), m. 229.degree. (from dioxane)] .lambda.max. in dioxane = 234 and 304 m.mu., log .epsilon., = 4.45 and 4.6, resp., orange-red color with $FeCl_3$. Pure ***trans*** -dihydrogeranic acid (9.0 g.) and 10 g. $SOCl_2$ after standing overnight and distg. gave the acid chloride, b12 88-90.degree.; to 30 g. in 40 cc. abs. Et_2O was added a soln. of $CdMe_2$ from 5 g. $CdCl_2$ and MeMgBr (from 1.2 g. Mg. and 5.0 g. MeBr) in abs. Et_2O during 40 min., the mixt. boiled 1.5 hrs., decompd. with ice and HCl, and extd. with Et_2O to give 1.9 g. methyl ***trans*** -2,2,6-trimethylcyclohexyl ketone (II), b12 86.degree. (no deriv. with semicarbazide or phenylsemicarbazide). II (1.9 g.) with 1.5 g. Ac_2O and BF_3 after 1 hr. gave 1.3 g. .beta.'-keto-**trans**-tetrahydroionone, b0.01 88.degree., .lambda.max. in alc. = 282 m.mu., log .epsilon. = 4.2 (monophenylsemicarbazone, m. 187-9.degree., .lambda.max. in alc. = 247 and 298 m.mu., log .epsilon. = 4.4 and 3.85, resp.). 3,4-Epoxy-.alpha.-ionone (III), b0.2 80.degree. (phenylsemicarbazone, m. 196.degree., .lambda.max. in alc. = 233 and 277 m.mu., log .epsilon. = 4.4 and 4.5, resp.), with Pd-$BaCO_3$ and H gave 3,4-epoxydihydro-.alpha.-ionone (IV), b0.1 78-91.degree., n_{22D} 1.4712 (phenylsemicarbazone, m. 167.degree., .lambda.max. in alc. = 248 m.mu., log .epsilon. = 4.4). After standing 3 days with 5 cc. 20% H_2SO_4 and 15 cc. alc., 0.5 g. IV gave a product $C_{13}H_{22}O_2$, b12 135.degree. (bath temp.), n_{22D} 1.4930 (strong $C(NO_2)_4$, but no carbonyl reactions), to which the cyclized structure 2,5,5,8a-tetramethyl-8-hydroxy-4a,5,6,7,8,8a-hexahydro-1,4H-benzopyran was given. IV (5 g.) in 20 cc. AcOH with 2 moles H and 0.4 g. PtO_2 gave a glassy residue, which in $CHCl_3$, treated with petr. ether till cloudy, gave 0.4 g. cryst. 4-ketotetrahydroionol (V), m. 129.degree., which also was obtained from III directly. V (0.10 g.) in 10 cc. AcOH with 0.10 g. CrO_3 in 10 cc. AcOH after standing overnight gave 4-ketotetrahydroionone (VI), b0.05 105.degree. (bath temp.) [bis(phenylsemicarbazone), m. 207-8.degree., .lambda.max. in dioxane = 247 m.mu., log .epsilon. = 4.8]; VI gave a large m.p. depression with I bis(phenylsemicarbazone). VI was also obtained from the noncryst. reduction product of V. Treatment of 0.45 g. VI with 1.0 g. $H_2NNH_2.H_2O$ and 0.7 g. Na in 15 cc. abs. EtOH 8 hrs. in a bomb tube at 200.degree. gave a hydrocarbon whose infrared spectrum is identical with that of authentic **trans**-tetrahydroionan. .alpha.',.beta.'-Epoxy-.alpha.-ionone (VII), m. 58.degree., (8 g.) (C.A. 41, 2017e) (phenylsemicarbazone, m. 176.degree. (from $CHCl_3$-MeOH), .lambda.max. in alc. = 253 m.mu., log .epsilon. = 4.25) with Pd-$BaCO_3$ and H absorbed 1 mole of H to give 3.1 g. colorless needles of .beta.'-hydroxydihydro-.alpha.-ionone (VIII), m. 63.degree. (from petr. ether), which gave no color with $FeCl_3$, a yellow with $C(NO_2)_4$ (phenylsemicarbazone (IX), m. 161.degree., .lambda.max. in alc. = 248, log .epsilon. = 4.45; 3,5-dinitrobenzoate, m. 138.degree. (from $CHCl_3$-MeOH)). VIII (0.5 g.) after 4 days in 5 cc. 20% H_2SO_4 and 15 cc. alc. gave .alpha.-ionone phenylsemicarbazone. Distn. of the oil from the reduction of VII gave .alpha.'-hydroxydihydro-.alpha.-ionone, b0.1 77-80.degree. (color with $FeCl_3$ and $C(NO_2)_4$) (phenylsemicarbazone, m. 171.degree., .lambda.max. in alc. = 253 m.mu., log .epsilon. = 4.45, gave a large depression of m.p. with IX).

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=> s l4 and (perfum? or fragran? or odor? or scent? or smell or olfactor?)
         29499 PERFUM?
         11493 FRAGRAN?
         74735 ODOR?
          2194 SCENT?
          4030 SMELL
           491 SMELLS
          4424 SMELL
                 (SMELL OR SMELLS)
         15268 OLFACTOR?
L6          32 L4 AND (PERFUM? OR FRAGRAN? OR ODOR? OR SCENT? OR SMELL OR OLFAC
               TOR?)

=> d l6 1-32 hitstr, ibib, iabs

L6   ANSWER 1 OF 32  CAPLUS  COPYRIGHT 2003 ACS on STN
IT   172462-28-1
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
        (perfume compds. for controlled release of active mols.)
RN   172462-28-1  CAPLUS
CN   2-Buten-1-one, 1-[(1R,3S,6S)-2,2,3,6-tetramethylcyclohexyl]-, (2E)-rel-
     (9CI)  (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.
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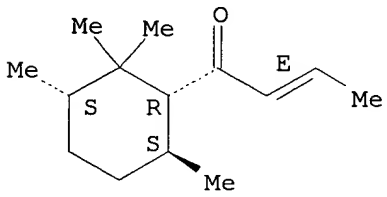


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IT   543724-38-5P
     RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (perfume compds. for controlled release of active mols.)
RN   543724-38-5  CAPLUS
CN   1-Butanone, 3-(benzoyloxy)-1-[(1R,3S,6S)-2,2,3,6-tetramethylcyclohexyl]-,
     rel- (9CI)  (CA INDEX NAME)

Relative stereochemistry.
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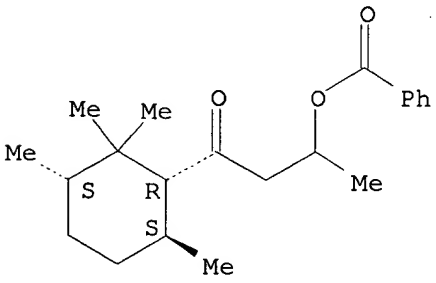


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IT   543724-39-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (perfume compds. for controlled release of active mols.)
RN   543724-39-6  CAPLUS
CN   1-Butanone, 3-(phenylmethoxy)-1-[(1R,3S,6S)-2,2,3,6-tetramethylcyclohexyl]-
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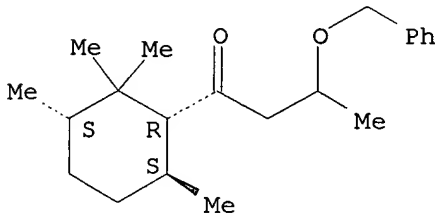
, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

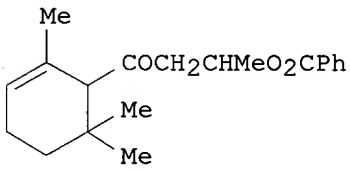


ACCESSION NUMBER: 2003:472328 CAPLUS
DOCUMENT NUMBER: 139:41490
TITLE: **Perfume** compounds for controlled release of active molecules
INVENTOR(S): Fehr, Charles; Struillou, Arnaud; Galindo, Jose
PATENT ASSIGNEE(S): Firmenich Sa, Switz.
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003049666	A2	20030619	WO 2002-IB5365	20021211

W: AU, BR, CA, CN, ID, IN, JP, MX, PL, RU, US, ZA
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR

PRIORITY APPLN. INFO.: WO 2001-IB2520 A 20011213
OTHER SOURCE(S): MARPAT 139:41490
GRAPHIC IMAGE:

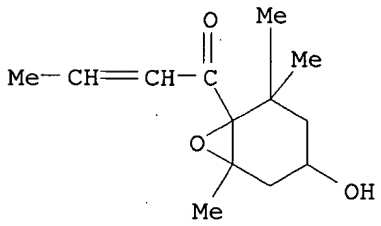


I

ABSTRACT:
The present invention relates to the field of **perfumery**. More particularly, it concerns compds. comprising at least one .beta.-oxy or .beta.-thio carbonyl moiety capable of liberating a **perfuming** mol. such as, for example, an .alpha.,.beta.-unsatd. ketone, aldehyde or carboxylic ester. The present invention concerns also the use of said compds. in ***perfumery*** as well as the **perfuming** compns. or ***perfumed*** articles comprising the invention's compds. Among many compds. prepd. were I and a random copolyer of 1-methyl-3-oxo-3-(2,6,6-trimethyl-3-cyclohexen-1-yl)propyl 4-vinylbenzoate and 4-vinylbenozic acid.

L6 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **172705-14-5**, 3-Hydroxy-5,6-epoxy-.beta.-ionol
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(aroma generation in lulo (Solanum quitoense) in relation to enzymic

hydrolysis of glycosides from leaves)
RN 172705-14-5 CAPLUS
CN 2-Buten-1-one, 1-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-(9CI) (CA INDEX NAME)

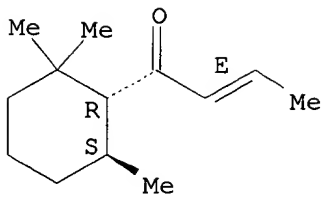


ACCESSION NUMBER: 2003:224778 CAPLUS
DOCUMENT NUMBER: 139:51953
TITLE: Studies on aroma generation in lulo (Solanum quitoense): enzymatic hydrolysis of glycosides from leaves
AUTHOR(S): Osorio, Coralia; Duque, Carmenza; Batista-Viera, Francisco
CORPORATE SOURCE: Departamento de Quimica, Universidad Nacional de Colombia, Bogota, AA 14490, Colombia
SOURCE: Food Chemistry (2003), 81(3), 333-340
CODEN: FOCHDJ; ISSN: 0308-8146
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
Five C13-norisoprenoid glycosides, isolated from lulo (Solanum quitoense) leaves, were subjected to enzymic hydrolysis with a com. glucosidase (emulsin) and also with an enzymic prepn. having glycosidase activity, isolated from lulo fruit pulp. The volatile compds. generated after reaction were characterized by capillary GC and capillary GC-MS. Lulo fruit glycosidases were extd. by ammonium sulfate pptn. at pH 6.5 and subjected to fractionation by hydrophobic interaction chromatog. (HIC) on Ph Sepharose gel, and some of their properties were detd. As the result of enzymic hydrolysis with exogenous enzymes (emulsin), glycosides isolated from lulo leaves produced only the aglycon (glycosidically bound volatile); in contrast, enzymic hydrolysis of glycosides, using endogenous enzymes (lulo fruit glycosidases), generated addnl. volatile compds., some recognizable as components of fruit flavor. The role of lulo leaf glycosides as flavor precursors was confirmed.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

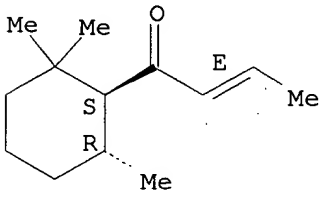
L6 ANSWER 3 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **146726-21-8P 146726-25-2P 379688-80-9P 379688-87-6P**
RL: COS (Cosmetic use); FFD (Food or feed use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and **odor** of trimethylcyclohexyl ketones via cationic olefin cyclization, stereoselective aldol condensation, and stereoselective oxidn.)
RN 146726-21-8 CAPLUS
CN 2-Buten-1-one, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



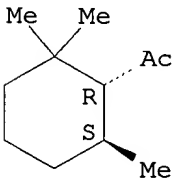
RN 146726-25-2 CAPLUS
CN 2-Buten-1-one, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



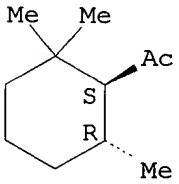
RN 379688-80-9 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



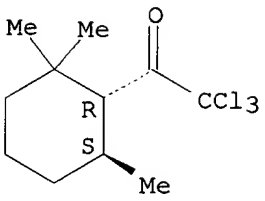
RN 379688-87-6 CAPLUS
CN Ethanone, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **409332-50-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and **odor** of trimethylcyclohexyl ketones via cationic olefin cyclization, stereoselective aldol condensation, and stereoselective oxidn.)
RN 409332-50-9 CAPLUS
CN Ethanone, 2,2,2-trichloro-1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

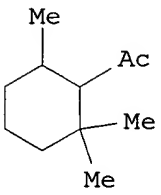


Applicant

ACCESSION NUMBER: 2003:28749 CAPLUS
DOCUMENT NUMBER: 138:368540
TITLE: Synthesis and **odor** of optically active trans-2,2,6-trimethylcyclohexyl methyl ketones and their related compounds
AUTHOR(S): Yamamoto, Takeshi; Ujihara, Hideo; Watanabe, Shinya; Harada, Makoto; Matsuda, Hiroyuki; Hagiwara, Toshimitsu
CORPORATE SOURCE: Central Research Laboratory, Takasago International Corporation, Hiratsuka, Kanagawa, 254-0073, Japan
SOURCE: Tetrahedron (2003), 59(4), 517-524
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:368540
ABSTRACT:
The syntheses of (1R,6S)-and (1S,6R)-2,2,6-trimethylcyclohexyl Me ketones (I) and (II) via cationic olefin cyclizations of ketone enol esters and their ***odor*** is described. (E)-(1R,6S)-and(E)-(1S,6R)-1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one were prepd. via stereoselective aldol condensation of I and II, followed by dehydration. (1R,6S)-Et 2,2,6-trimethylcyclohexylcarboxylate was prepd. via stereoselective oxidn. of I.

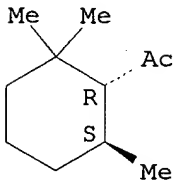
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **26383-28-8**, 2,2,6-Trimethylcyclohexyl methyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of 2,2,6-trimethylcyclohexanecarboxylic acid by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone by HNO3)
RN 26383-28-8 CAPLUS
CN Ethanone, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



IT **379688-80-9P**, (1R,6S)-2,2,6-Trimethylcyclohexyl methyl ketone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 2,2,6-trimethylcyclohexanecarboxylic acid by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone by HNO3)
RN 379688-80-9 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



Applicants

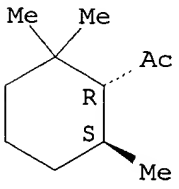
ACCESSION NUMBER: 2002:126357 CAPLUS
DOCUMENT NUMBER: 136:167525
TITLE: Preparation of 2,2,6-trimethylcyclohexanecarboxylic acid from 2,2,6-trimethylcyclohexyl methyl ketone
INVENTOR(S): Harada, Mutsumi; Matsuda, Hiroyuki; Ujihara, Hideo; Watabe, Shinya; Yamamoto, Takeshi
PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002053520	A2	20020219	JP 2000-242570	20000810

PRIORITY APPLN. INFO.: JP 2000-242570 20000810
OTHER SOURCE(S): CASREACT 136:167525
ABSTRACT:
2,2,6-Trimethylcyclohexanecarboxylic acid (I), useful as an intermediate for ***fragrant*** substances, is prepd. by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone (II). Thus, (1R,6S)-II was oxidized by HNO3 at 90.degree. for 3 h in H2O to give 98% (1R,6S)-I.

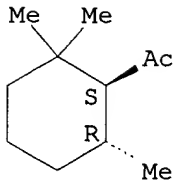
L6 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **379688-80-9P**, (1R,6S)-2,2,6-Trimethylcyclohexyl methyl ketone
379688-87-6P, (1S,6R)-2,2,6-Trimethylcyclohexyl methyl ketone
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in **perfumes** and colognes)
RN 379688-80-9 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



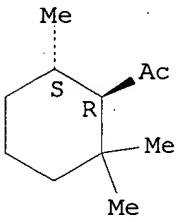
RN 379688-87-6 CAPLUS
CN Ethanone, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



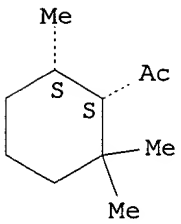
IT **52842-33-8DP**, trans-2,2,6-Trimethylcyclohexyl methyl ketone, chiral
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in **perfumes** and colognes)
RN 52842-33-8 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



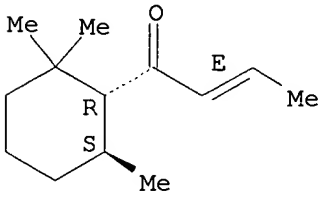
IT **52612-52-9P**, (1S,6S)-2,2,6-Trimethylcyclohexyl methyl ketone **146726-21-8P**, trans-[(1R,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-22-9P**, cis-[(1S,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-23-0P**, trans-[(1R,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one **146726-24-1P**, cis-[(1S,6S)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one **146726-25-2P**, trans-[(1S,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-26-3P**, cis-[(1R,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2E)-2-buten-1-one **146726-27-4P**, trans-[(1S,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one **146726-28-5P**, cis-[(1R,6R)-1-(2,2,6-Trimethylcyclohexyl)]-(2Z)-2-buten-1-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in **perfumes** and colognes)
RN 52612-52-9 CAPLUS
CN Ethanone, 1-(2,2,6-trimethylcyclohexyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



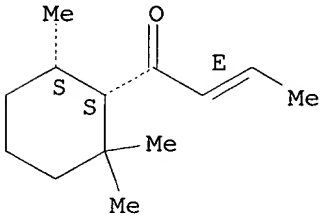
RN 146726-21-8 CAPLUS
CN 2-Buten-1-one, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



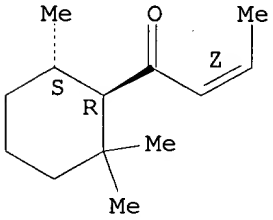
RN 146726-22-9 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(E),6.alpha.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



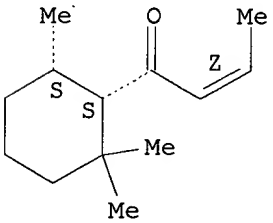
RN 146726-23-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.beta.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



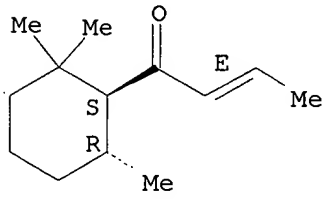
RN 146726-24-1 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.alpha.]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



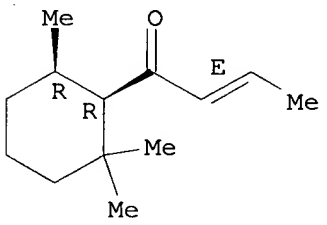
RN 146726-25-2 CAPLUS
CN 2-Buten-1-one, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



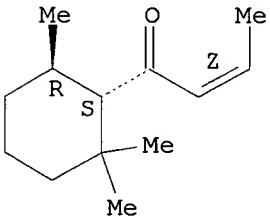
RN 146726-26-3 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(E),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



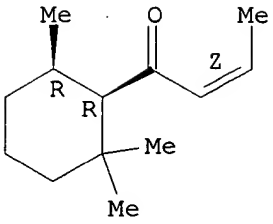
RN 146726-27-4 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-28-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

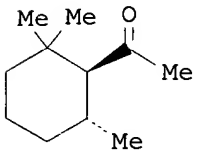


Applicant

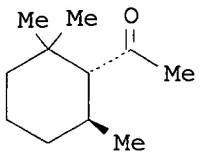
ACCESSION NUMBER: 2001:900121 CAPLUS
DOCUMENT NUMBER: 136:37794
TITLE: Process for producing (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl methyl ketone and **perfume** compositions containing them
INVENTOR(S): Ujihara, Hideo; Watanabe, Shinya; Yamamoto, Takeshi; Toshimitsu, Hagiwara
PATENT ASSIGNEE(S): Takasago International Corporation, Japan
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1162191	A2	20011212	EP 2001-401473	20010607
EP 1162191	A3	20020904		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001348353	A2	20011218	JP 2000-170822	20000607
US 2002042356	A1	20020411	US 2001-876883	20010607

PRIORITY APPLN. INFO.: JP 2000-170822 A 20000607
OTHER SOURCE(S): CASREACT 136:37794
GRAPHIC IMAGE:



I



II

ABSTRACT:
A process for producing trans-2,2,6-trimethylcyclohexyl Me ketone, which is the (1S,6R)-2,2,6-trimethylcyclohexyl Me ketone (I) and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone (II), is described. Thus, I was prepd. from (R)-citronellol via condensation with EtMgBr in THF, Jones oxidn. in MeCOMe, acetylation with isopropenyl acetate contg. p-MeC6H4SO3H and cyclization with 85% H3PO4 in PhMe. A unique, novel eucalyptus, mint-like and white floral ***perfume*** material can be provided using the ketone compds. disclosed in the present invention as well by the prodn. process disclosed therein.

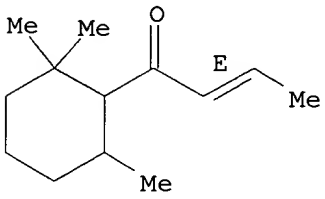
L6 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **359865-02-4P**
RL: BUU (Biological use, unclassified); FFD (Food or feed use); SPN

(Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of damascone or damascenone by simultaneous catalytic oxidn. and redn. of damascol and damascenol)

RN 359865-02-4 CAPLUS

CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (2E)- (9CI) (CA INDEX NAME)

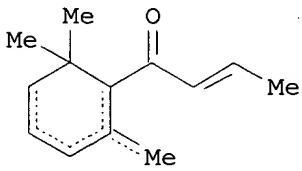
Double bond geometry as shown.



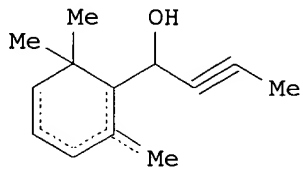
ACCESSION NUMBER: 2001:664522 CAPLUS
DOCUMENT NUMBER: 135:242372
TITLE: Method for preparation of damascone or damascenone by simultaneous catalytic oxidation and reduction of damascol and damascenol
INVENTOR(S): Watanabe, Kazunori
PATENT ASSIGNEE(S): Nippon Zeon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001247504	A2	20010911	JP 2000-60171	20000306

PRIORITY APPLN. INFO.: JP 2000-60171 20000306
OTHER SOURCE(S): CASREACT 135:242372; MARPAT 135:242372
GRAPHIC IMAGE:



I

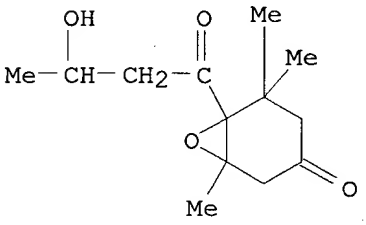


II

ABSTRACT:
.alpha., .beta., .gamma.-Damascone and damascenone [I; wherein the dotted lines represent (1) one carbon-carbon double is present at 1, 2, or 3-position of the six-membered ring which possesses Me group at 2-position; (2) no carbon-carbon double bond is present in the six-membered ring which possesses Me group at 2-position; (3) two carbon-carbon double bonds are present at 1 and 3 or 2 and 4 positions in the six -membered ring which possesses Me group at 2-position; and (4) one carbon-carbon double bond is present in the six-membered ring which possesses Me group at 2-position] are prepd. by contacting dehydro-.alpha., .beta., .gamma.-damascol and damascenol (II; wherein the dotted lines are defined as above) with a palladium complex catalyst. This process eliminates sep. oxidn. and redn. steps of prior art methods and gives in short steps damascone or damascenone I which possess fruit or flower-like **fragrance**

or taste and are useful as flavoring materials for food or cosmetics. Thus, 100 mg dehydro-.beta.-damascol, which was prepd. from .beta.-cyclocitral, was dissolved in 2 mL PhMe, treated with 5 mol% Pd(OAc)2 and 35 mol% Ph3P, and stirred at 80.degree. for 5 h to give 49% .beta.-damascone.

L6 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **257941-12-1**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(aroma characterization of Sardinian strawberry tree (Arbutus unedo) honey)
RN 257941-12-1 CAPLUS
CN 7-Oxabicyclo[4.1.0]heptan-3-one, 6-(3-hydroxy-1-oxobutyl)-1,5,5-trimethyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1999:599211 CAPLUS
DOCUMENT NUMBER: 132:150899
TITLE: Aroma characterization of Sardinian strawberry tree (Arbutus unedo L.) honey
AUTHOR(S): Dalla Serra, A.; Franco, M. A.; Mattivi, F.; Ramponi, M.; Vacca, V.; Versini, G.
CORPORATE SOURCE: Laboratorio di Analisi e Ricerche, Centro Sperimentale, Istituto Agrario di San Michele all'Adige, Trento, 38100, Italy
SOURCE: Italian Journal of Food Science (1999), 11(1), 47-56
CODEN: ITFSEY; ISSN: 1120-1770
PUBLISHER: Chiriotti Editori spa
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:
Gas chromatog.-mass spectrometric (GC-MS) anal. of the aroma fraction isolated from several strawberry tree blossom honey samples showed a marked predominance of norisoprenoids. Some were identified or tentatively identified as C9, C10, and C13 compds. For this aspect, the honey is similar to that from another plant of the Ericaceae family, heather, but is distinguishable from it due to different concns. of the compds. common to both and the uniqueness of several substances, whose tentative structures have been attributed with the support of GC-Fourier Transform IR (FTIR) spectra. Some interesting C10 aldehyde structures are proposed. Most compds. could be interrelated in degrdn. processes, starting from the compds. with the highest mol. wt. Among the samples from different areas of Sardinia, there were important quant. differences in some of the most abundant compds.

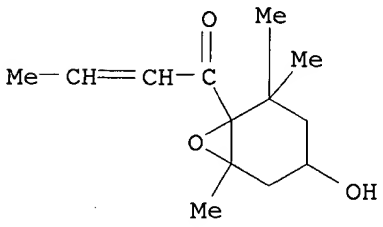
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **172705-14-5**, 3-Hydroxy-5,6-epoxy-.beta.-ionol
RL: BOC (Biological occurrence); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence); PROC (Process)

(effect of sun exposure on carotenoids and C13-norisoprenoid glycosides in Syrah berries (Vitis vinifera))

RN 172705-14-5 CAPLUS

CN 2-Buten-1-one, 1-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-(9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1998:741154 CAPLUS
DOCUMENT NUMBER: 130:138573
TITLE: Effect of sun exposure on carotenoids and C13-norisoprenoid glycosides in Syrah berries (Vitis vinifera L.)
AUTHOR(S): Razungles, Alain J.; Baumes, Raymond L.; Dufour, Claire; Sznaper, Clara N.; Bayonove, Claude L.
CORPORATE SOURCE: ENSAM - Inra - Institut des produits de la vigne - ISVVM, Laboratoire des aromes et substances naturelles, 2, Montpellier, 34060, Fr.
SOURCE: Sciences des Aliments (1998), 18(4), 361-373
CODEN: SCALDC; ISSN: 0240-8813
PUBLISHER: Lavoisier Abonnements
DOCUMENT TYPE: Journal
LANGUAGE: English
ABSTRACT:

Carotenoids are considered precursors of C13-norisoprenoids in grape berries. The latter compds. can play an important role in the organoleptic quality of wines because their compn. influences flavors and aromas. Sunlight effect on the berry carotenoid and C13-norisoprenoid compns. was studied before and after veraison. Syrah berries which were sun-exposed before veraison were found to be richer in carotenoids than shaded berries. However, after veraison, sunlight caused the degrdn. of these pigments. Sunlight modified the nonepoxyxanthophyll/epoxyxanthophyll ratios. Metabolic relationships between the glycosylated C13-norisoprenoids and their potential precursors were tentatively established between certain C13-norisoprenoids and carotenoids in specific sun-exposure treatments. In addn., the sunlight effect on the rise of other glycosidically bound compds. such as monoterpenes and phenols was evidenced.

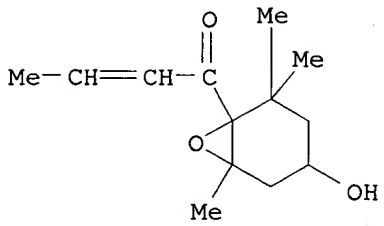
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN

IT **172705-14-5P**, 3-Hydroxy-5,6-epoxy-.beta.-ionol
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(product of enzymic hydrolysis of Solanum quitoense leaf glycosides)

RN 172705-14-5 CAPLUS

CN 2-Buten-1-one, 1-(4-hydroxy-2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-(9CI) (CA INDEX NAME)

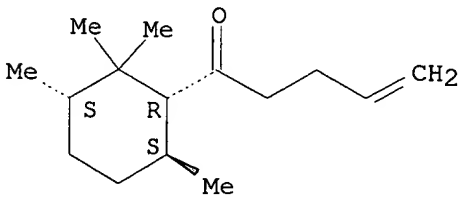


ACCESSION NUMBER: 1996:627334 CAPLUS
DOCUMENT NUMBER: 125:297034
TITLE: Volatiles generated by enzymic hydrolysis of glycosides from Solanum quitoense leaves
AUTHOR(S): Osorio R., Coralia; Duque B., Carmenza
CORPORATE SOURCE: Departamento Quimica, Universidad Nacional Colombia, AA. 14490, Czech.
SOURCE: Revista Colombiana de Quimica (1995), 24(2), 69-81
CODEN: RCLQAY; ISSN: 0120-2804
PUBLISHER: Universidad Nacional de Colombia, Departamento de Quimica
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
ABSTRACT:

HRGC (High Resoln. Gas Chromatography), HRGC-MS (High Resoln. Gas Chromatog.-Mass Spectrometry) identification and HRGC-vs-sniffing sensory anal. (**odor** description) of glycoside-bound volatiles from S. quitoense leaves were carried out after isolation of an ext. obtained by Amberlite XAD-2 adsorption and methanol elution followed by enzymic hydrolysis with a nonselective glycosidase (Rohapect D5- L). In total, 25 volatiles were detected, of which 21 were pos. identified (about 90% of the total aglycons). C13-Norisoprenoids afforded the most abundant group of compds. (38.1%, 15 mg/kg leaves), followed by arom. compds. (30.5%), monoterpene alcs. (12.3%), and C6-aliph. compds. (9.3%). The bulk of volatiles produced by enzymic hydrolysis possessed a pleasant green woody aroma with strong sweet honey note.

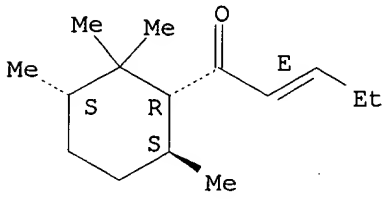
L6 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **172462-13-4P 172462-14-5P 172462-15-6P**
172462-17-8P 172462-18-9P 172462-22-5P
172462-23-6P 172462-24-7P 172462-25-8P
172462-26-9P 172462-27-0P 172462-28-1P
172462-29-2P 172586-25-3P 172586-26-4P
172586-27-5P 172586-28-6P 172586-29-7P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of 1-cyclohex(en)ylalkan- and -en-1-ones as **perfume fragrances**)
RN 172462-13-4 CAPLUS
CN 4-Penten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



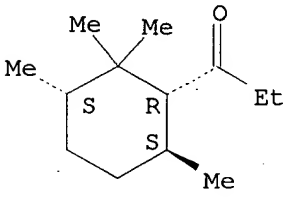
RN 172462-14-5 CAPLUS
CN 2-Penten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, [1.alpha.(E),3.alpha.,6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



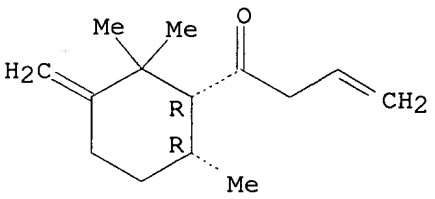
RN 172462-15-6 CAPLUS
CN 1-Propanone, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



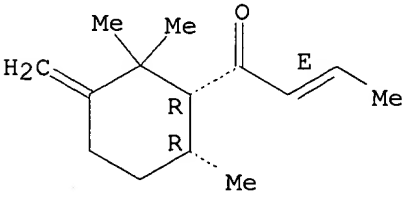
RN 172462-17-8 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

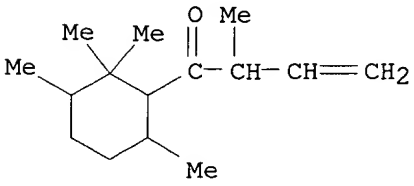


RN 172462-18-9 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, [1.alpha.(E),6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

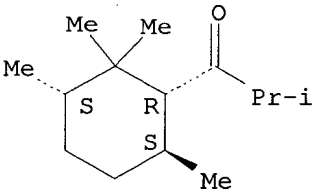


RN 172462-22-5 CAPLUS
CN 3-Buten-1-one, 2-methyl-1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



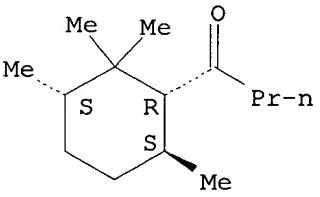
RN 172462-23-6 CAPLUS
CN 1-Propanone, 2-methyl-1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

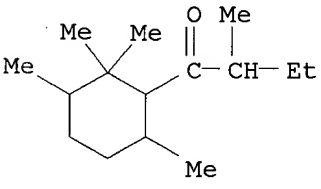


RN 172462-24-7 CAPLUS
CN 1-Butanone, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

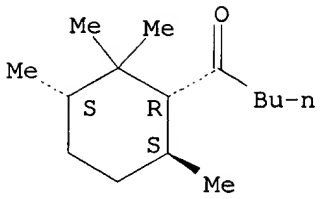


RN 172462-25-8 CAPLUS
CN 1-Butanone, 2-methyl-1-(2,2,3,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



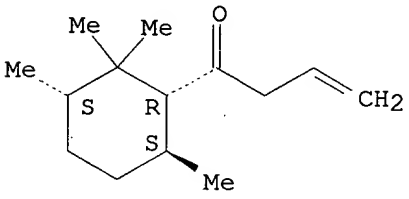
RN 172462-26-9 CAPLUS
CN 1-Pentanone, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



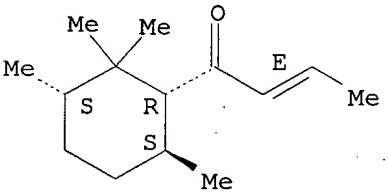
RN 172462-27-0 CAPLUS
CN 3-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



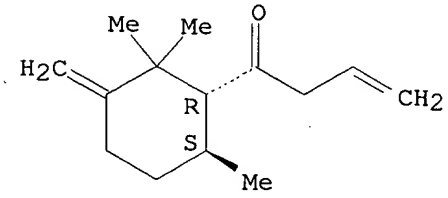
RN 172462-28-1 CAPLUS
CN 2-Buten-1-one, 1-[(1R,3S,6S)-2,2,3,6-tetramethylcyclohexyl]-, (2E)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



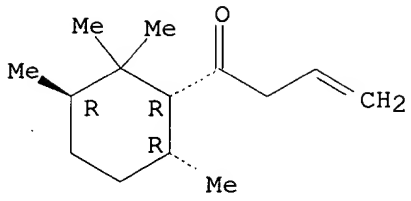
RN 172462-29-2 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



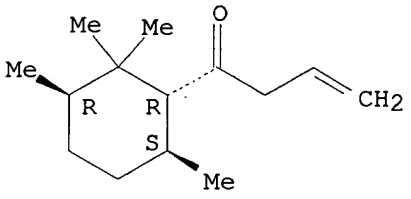
RN 172586-25-3 CAPLUS
CN 3-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.beta.,6.alpha.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



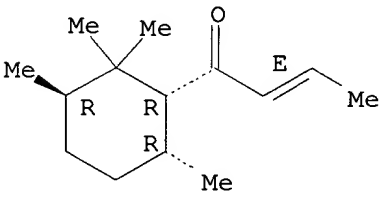
RN 172586-26-4 CAPLUS
CN 3-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, (1.alpha.,3.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



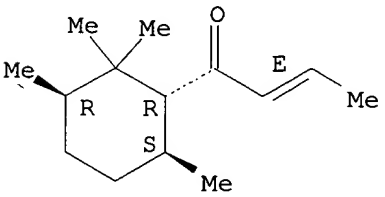
RN 172586-27-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, [1.alpha.(E),3.beta.,6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



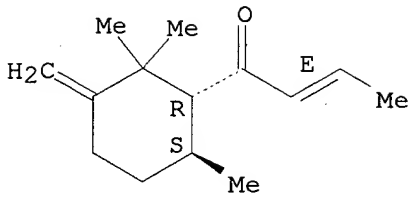
RN 172586-28-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,3,6-tetramethylcyclohexyl)-, [1.alpha.(E),3.beta.,6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 172586-29-7 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-3-methylenecyclohexyl)-, [1.alpha.(E),6.beta.]- (9CI) (CA INDEX NAME)

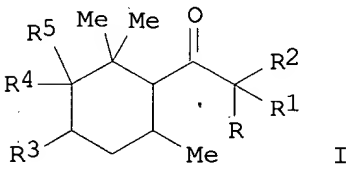
Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1995:994742 CAPLUS
DOCUMENT NUMBER: 124:86432
TITLE: Preparation of 1-cyclohex(en)ylalkan- and -en-1-ones as **perfume fragrances**
INVENTOR(S): Schulte-Elte, Karl-Heinrich; Chapuis, Christian; Pamingle, Herve; Blanc, Pierre-Alain
PATENT ASSIGNEE(S): Firmenich S. A., Switz.
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 676393	A1	19951011	EP 1995-103729	19950315
EP 676393	B1	19980819		

R: CH, DE, FR, GB, LI, NL
PRIORITY APPLN. INFO.: CH 1994-1047 19940408
OTHER SOURCE(S): MARPAT 124:86432
GRAPHIC IMAGE:

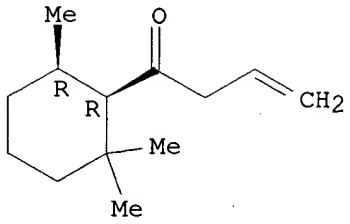


I

ABSTRACT:
Title compds. [I; R = H or Me; R1 = H, alk(en)yl; R2-R4 = H; R1R2 = alkylidene; R3R4 = bond; R5 = Me; R4R5 = CH2] were prepd. Thus, 2,2,3,6-tetramethyl-3-cyclohexene-1-carboxaldehyde was condensed with EtMgBr and the product oxidized to give cis-1-(2,2,3,6-tetramethyl-3-cyclohexen-1-yl)-1-propanone. ***Perfume*** formulations comprising I were given.

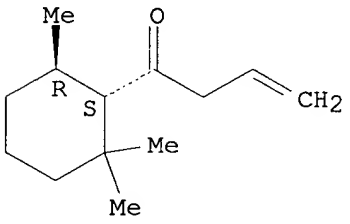
L6 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **146726-38-7P 146726-39-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of methylcyclohexylbutenone flavoring agent)
RN 146726-38-7 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



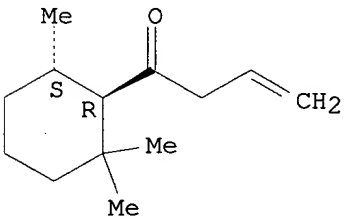
RN 146726-39-8 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



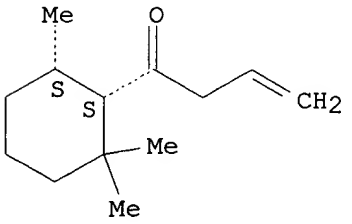
IT **146657-22-9P 146726-32-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of)
RN 146657-22-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 146726-32-1 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, (1S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

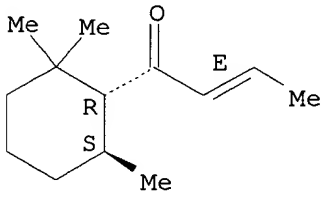


IT **146726-21-8P 146726-22-9P 146726-23-0P**

146726-24-1P 146726-25-2P 146726-26-3P
146726-27-4P 146726-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as flavoring agent)

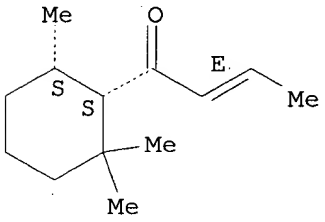
RN 146726-21-8 CAPLUS
CN 2-Buten-1-one, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



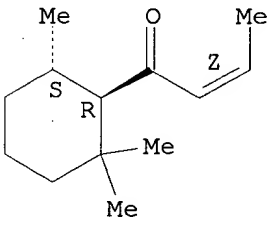
RN 146726-22-9 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(E),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



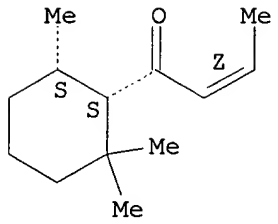
RN 146726-23-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



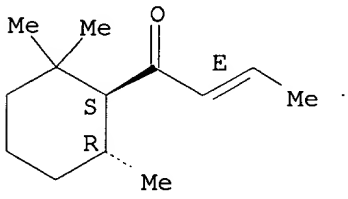
RN 146726-24-1 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



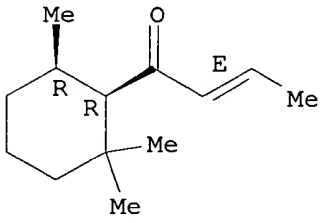
RN 146726-25-2 CAPLUS
CN 2-Buten-1-one, 1-[(1S,6R)-2,2,6-trimethylcyclohexyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



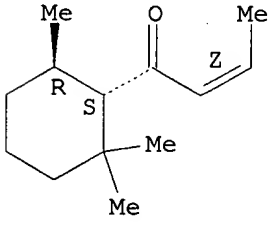
RN 146726-26-3 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(E),6.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-27-4 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1S-[1.alpha.(Z),6.beta.]]- (9CI) (CA INDEX NAME)

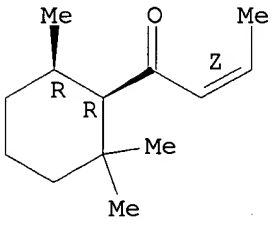
Absolute stereochemistry.
Double bond geometry as shown.



RN 146726-28-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1R-[1.alpha.(Z),6.alpha.]]-

(9CI) (CA INDEX NAME)

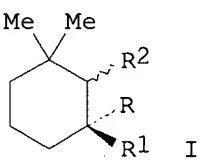
Absolute stereochemistry.
Double bond geometry as shown.



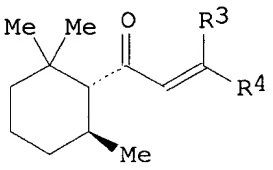
ACCESSION NUMBER: 1993:254447 CAPLUS
DOCUMENT NUMBER: 118:254447
TITLE: Preparation of optically active 1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one compounds as flavor compositions
INVENTOR(S): Shimada, Akiyoshi; Omoto, Tatsuya; Yamamoto, Takeshi
PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04330033	A2	19921118	JP 1990-236980	19900910
JP 2748184	B2	19980506		

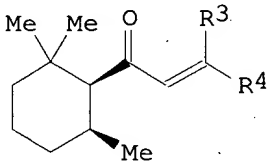
PRIORITY APPLN. INFO.: JP 1990-236980 19900910
OTHER SOURCE(S): CASREACT 118:254447
GRAPHIC IMAGE:



I



II

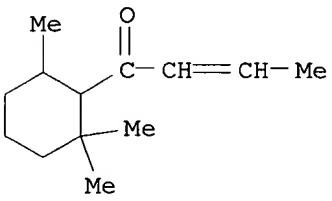


III

ABSTRACT:
The title compds. (I; R = H, R1 = Me; R = Me, R1 = H; R2 = COCH:CHMe), having fruit-like flavor, are prepd. A flavor compn. contg. I is used for foods, beverages, cosmetics, flavoring agents, and sanitation materials. Thus, (6S)-I (R = H, R1 = Me, R2 = CHO)(prepn. given) 100, allyl bromide 120, Zn powder 83 g, 200 mL DMF were stirred at room temp. for 4 h to give 83% (6S)-I [R = H, R1 = Me, R2 = CH(OH)CH2CH:CH2] as a mixt. trans-threo-, trans-erythro-, cis-threo-, cis-erythro-isomers which (104 g) was oxidized with Cr3O in aq. acetone contg. H2SO4 at 20-25.degree. to give 91% I (R = H, R1 = Me, R2 =

COCH2CH:CH2) contg. 91% trans-isomer and 9% cis-isomer. This (95 g) was heated with 4.8 g p-Me6H4SO3H in PhMe for isomerization at 80.degree. for 30 min to give (6S)-I (R = H, R1 = Me, R2 = COCH:CHMe) contg. trans-(E)-isomer II (R3 = H, R4 = Me) 87.2, cis-(E)-isomer III (R3 = H, R4 = Me) 8.4, trans-(Z)-isomer II (R3 = Me, R4 = H) 4.0, and cis-(Z)-isomer III (R3 = Me, R4 = H) 0.3% which showed strong diffusion property and ripe fruit-like flavor with rose petal-like warm flowery flavor. (6R)-I (R = H, R1 = Me, R2 = COCH:CHMe) was also prepd. and showed a camphor-like flavor as well as a fruit-like flavor with green apple tone, a stimulating green floral tone, or a .beta.-damascone-like tone.

L6 ANSWER 12 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **39900-18-0D**, derivs.
RL: BIOL (Biological study)
(**perfume** compns. contg. phenylethyl Me carbonate and)
RN 39900-18-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1984:428113 CAPLUS
DOCUMENT NUMBER: 101:28113
TITLE: Phenylethyl methyl carbonate, mixtures containing it and their organoleptic uses
INVENTOR(S): Boden, Richard M.; Tyszkiewicz, Theodore J.; Watkins, Hugh
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc. , USA
SOURCE: U.S., 14 pp. Division of U.S. Ser. No. 329,221.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

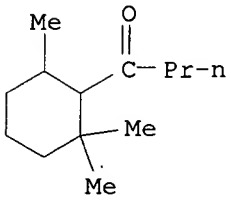
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4436652	A	19840313	US 1982-422489	19820923
US 4464280	A	19840807	US 1983-546390	19831028

PRIORITY APPLN. INFO.: US 1981-329221 19811210
US 1982-422489 19820923

ABSTRACT:
Perfumes and **perfumed** articles consist of a mixt. of phenylethyl methyl carbonate (I) [1796-66-3], 5-phenyl-3-methylpentanol isomers and 1 or more butenoylcyclohexane derivs. The mixt. may be used in hair sprays, shampoos, cosmetics, etc. Thus, I was prepd. by the condensation of phenylethyl acetate [103-45-7] and (MeO)2CO [616-38-6] in the presence of NaOMe. The use of I along with other ingredients in improving the **odor** of various formulations is given.

L6 ANSWER 13 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **76038-07-8P**
RL: PREP (Preparation)
(prepn. of, for **perfume** compns.)

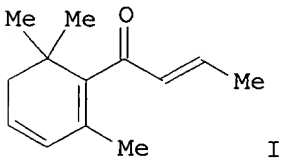
RN 76038-07-8 CAPLUS
CN 1-Butanone, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



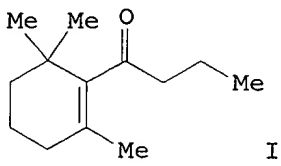
ACCESSION NUMBER: 1981:36129 CAPLUS
DOCUMENT NUMBER: 94:36129
TITLE: Hydrogenation of 2,6,6-trimethyl cyclohexene derivatives for organoleptic uses
INVENTOR(S): Trenkle, Robert Walter; Mookherjee, Braja Dulal; Schmitt, frederick Louis; Vock, Manfred Hugo; Vinals, Joaquin F.; Kiwala, Jacob
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA
SOURCE: Eur. Pat. Appl., 75 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 12436	A1	19800625	EP 1979-105144	19791213
EP 12436	B1	19821124		
R: CH, DE, FR, GB, NL				
US 4292447	A	19810929	US 1978-969852	19781215
US 4311754	A	19820119	US 1981-239051	19810227
US 4313842	A	19820202	US 1981-239049	19810227
US 4315953	A	19820216	US 1981-239048	19810227
US 4324704	A	19820413	US 1981-238680	19810227
US 4360032	A	19821123	US 1981-239052	19810227

PRIORITY APPLN. INFO.: US 1978-969852 19781215
GRAPHIC IMAGE:



I



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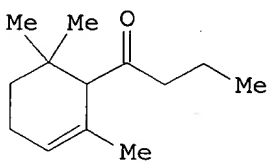
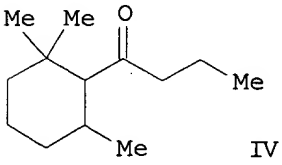
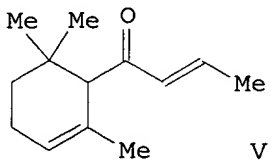


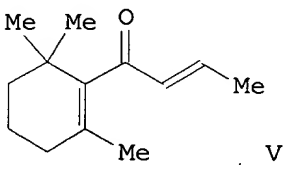
III



IV



V

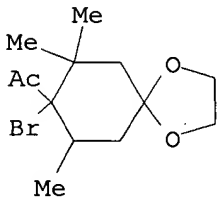


VI

ABSTRACT:
.beta.-Damascenone (I) [23726-93-4] was hydrogenated (H2/Pd/CuCO3) to give a mixt. of II [28384-26-1], III [28361-64-0], and IV [**76038-07-8**]. Using H2/Pd/BaSO4, I gave II, III, V [24720-09-0], and VI [23726-91-2] along with a cis-isomer of VI [23726-92-3] as an artifact formed as a result of

distn. These fractions from hydrogenation of I were added to **perfume** compns. to enhance the **fragrance** note. The **perfume** compns. were added to soap, detergent, shampoo, hair prepns. and, flavor formulations and as additives for tobacco.

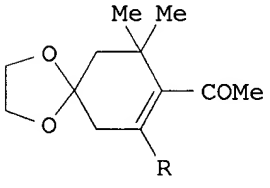
L6 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **71659-90-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydrobromination of)
RN 71659-90-0 CAPLUS
CN Ethanone, 1-(8-bromo-7,7,9-trimethyl-1,4-dioxaspiro[4.5]dec-8-yl)- (9CI) (CA INDEX NAME)



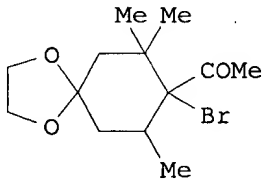
ACCESSION NUMBER: 1979:575321 CAPLUS
DOCUMENT NUMBER: 91:175321
TITLE: 1-Acetyl-4,4-ethylenedioxy-1-cyclohexenes
INVENTOR(S): Matsui, Masanao; Kitahara, Takeshi; Takagi, Keiichi
PATENT ASSIGNEE(S): Hasegawa, T., Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54048765	A2	19790417	JP 1977-114306	19770922
JP 60003308	B4	19850126		

PRIORITY APPLN. INFO.: JP 1977-114306 19770922
GRAPHIC IMAGE:



I

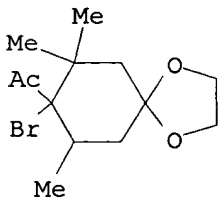


III

ABSTRACT:
Ketals I (R = H, Me), having floral aroma and useful as **perfume** components, were prepd. by heating MeOCH:CHC(OSiMe3):CH2 (II) with mesityl oxide, followed by ketalization and methylation via III. Thus, 100 g II, prepd. in 76% yield from 4-methoxy-3-buten-2-one, Et3N, ZnCl2, and Me3SiCl, were heated with 20 g mesityl oxide in an autoclave at 180.degree. for 20 h and the mixt. refluxed with ethylene glycol and p-MeC6H4SO3H in C6H6 to give 67% I (R = H). This (10.5 g) was added to Me2CuLi, prepd. from 15.0 g CuI and MeLi in Et2O, at 0.degree. and the mixt. treated with Br in C6H6 at -60.degree. to

give 88% III, also prepd. in 82% yield with MeMgI-CuI instead of Me2CuLi. III (12.2 g) heated with 4.2 g LiCl and 7.4 g Li2CO3 in DMF at 100.degree. for 20 h gave 78% I (R = Me), also prepd. in 68% yield with 1,8-diazabicyclo[5.8.0]undec-7-ene as the base.

L6 ANSWER 15 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **71659-90-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 71659-90-0 CAPLUS
CN Ethanone, 1-(8-bromo-7,7,9-trimethyl-1,4-dioxaspiro[4.5]dec-8-yl)- (9CI) (CA INDEX NAME)

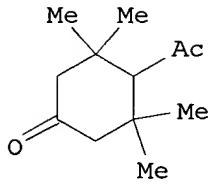


ACCESSION NUMBER: 1979:574903 CAPLUS
DOCUMENT NUMBER: 91:174903
TITLE: 4-Hydroxy-.beta.-damascon, .beta.-damascenone, and their dihydro compounds
INVENTOR(S): Matsui, Masanao; Kitahara, Takeshi; Takagi, Keiichi
PATENT ASSIGNEE(S): Hasegawa, T., Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

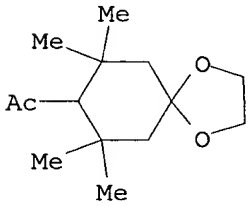
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54048738	A2	19790417	JP 1977-114308	19770922
JP 61005458	B4	19860218		

PRIORITY APPLN. INFO.: JP 1977-114308 19770922
ABSTRACT:
.beta.-Damascenone and dihydro-.beta.-damascenone (I) were prepd. from 4-hydroxy-.beta.-damascone (II), 4-hydroxydihydro-.beta.-damascone (III), or 1-crotonyl-2,6,6-trimethyl-1-cyclohexen-4-one. Thus, II in THF was reduced with LiAlH3(OCMe3) to give 17% unreacted II and 53% III. III reacted with MeSO2Cl in pyridine and the product treated with NaI and collidine to give 78% I.

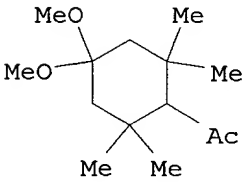
L6 ANSWER 16 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **16556-46-0P 16556-47-1P 16556-49-3P**
16556-57-3P 16556-58-4P 16556-59-5P
16556-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for **perfumes**)
RN 16556-46-0 CAPLUS
CN Cyclohexanone, 4-acetyl-3,3,5,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



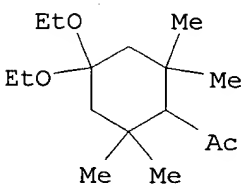
RN 16556-47-1 CAPLUS
CN Ethanone, 1-(7,7,9,9-tetramethyl-1,4-dioxaspiro[4.5]dec-8-yl)- (9CI) (CA INDEX NAME)



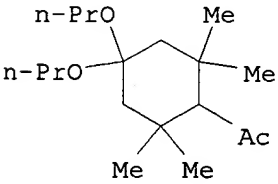
RN 16556-49-3 CAPLUS
CN Ethanone, 1-(4,4-dimethoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 16556-57-3 CAPLUS
CN Ethanone, 1-(4,4-diethoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)

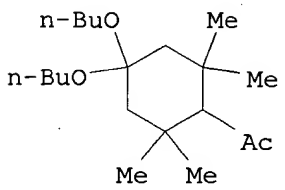


RN 16556-58-4 CAPLUS
CN Ethanone, 1-(2,2,6,6-tetramethyl-4,4-dipropoxycyclohexyl)- (9CI) (CA INDEX NAME)

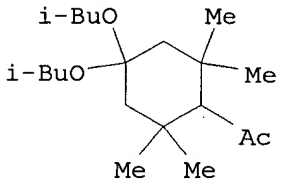


RN 16556-59-5 CAPLUS

CN Ethanone, 1-(4,4-dibutoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 16556-60-8 CAPLUS
CN Ethanone, 1-[2,2,6,6-tetramethyl-4,4-bis(2-methylpropoxy)cyclohexyl]- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1976:559521 CAPLUS
DOCUMENT NUMBER: 85:159521
TITLE: 4-Acetyl-3,3,5,5-tetraalkylcyclohexanones
INVENTOR(S): Corbier, Bernard P.; Teisseire, Paul J.
PATENT ASSIGNEE(S): Societe Anonyme Roure Bertrand Dupont, Fr.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3953515	A	19760427	US 1975-546531	19750203
US 3875241	A	19750401	US 1971-110652	19710128
US 3948815	A	19760406	US 1975-546564	19750203

PRIORITY APPLN. INFO.:
CH 1965-14216 19651014
US 1966-585269 19661010
US 1971-110652 19710128
US 1966-585259 19661010

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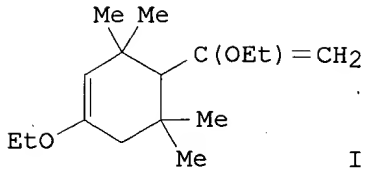
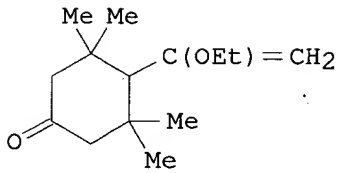


I



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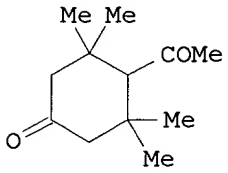
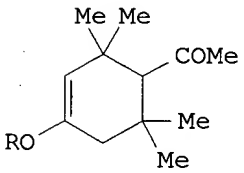
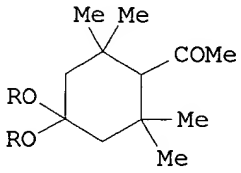


III



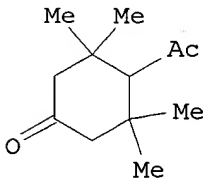
IV



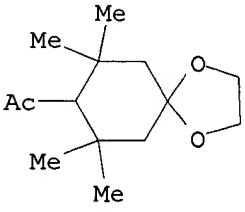
V

ABSTRACT:
Concurrent cyclodimerization of Me2C:CHCOMe and its reaction with HC(OEt)3 in the presence of BF3.Et2O gave a mixt. of I and II which was hydrolyzed to III. III with HC(OR)3 (R = Et, Pr, Bu, Me2CHCH2, amyl, isoamyl) in the presence of BF3.Et2O gave IV and V. The enol ethers and ketals are useful in ***perfumes*** .

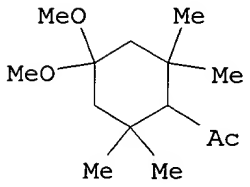
L6 ANSWER 17 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **16556-46-0P 16556-47-1P 16556-49-3P**
16556-57-3P 16556-58-4P 16556-59-5P
16556-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for **perfumes**)
RN 16556-46-0 CAPLUS
CN Cyclohexanone, 4-acetyl-3,3,5,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



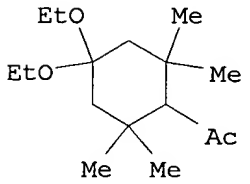
RN 16556-47-1 CAPLUS
CN Ethanone, 1-(7,7,9,9-tetramethyl-1,4-dioxaspiro[4.5]dec-8-yl)- (9CI) (CA INDEX NAME)



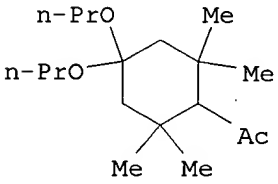
RN 16556-49-3 CAPLUS
CN Ethanone, 1-(4,4-dimethoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



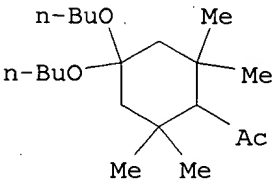
RN 16556-57-3 CAPLUS
CN Ethanone, 1-(4,4-diethoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



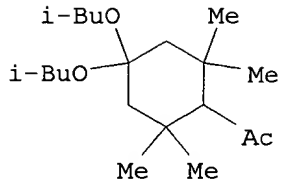
RN 16556-58-4 CAPLUS
CN Ethanone, 1-(2,2,6,6-tetramethyl-4,4-dipropoxycyclohexyl)- (9CI) (CA INDEX NAME)



RN 16556-59-5 CAPLUS
CN Ethanone, 1-(4,4-dibutoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 16556-60-8 CAPLUS
CN Ethanone, 1-[2,2,6,6-tetramethyl-4,4-bis(2-methylpropoxy)cyclohexyl]- (9CI) (CA INDEX NAME)

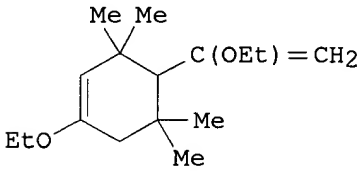


ACCESSION NUMBER: 1976:559520 CAPLUS
DOCUMENT NUMBER: 85:159520
TITLE: Mono-enol ethers of 4-acetyl-3,3,5,5-tetramethylcyclohexanone
INVENTOR(S): Corbier, Bernard P.; Teisseire, Paul J.
PATENT ASSIGNEE(S): Societe Anonyme Roure Bertrand Dupont, Fr.
SOURCE: U.S., 6 pp. Division of U.S. 3,875,241.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

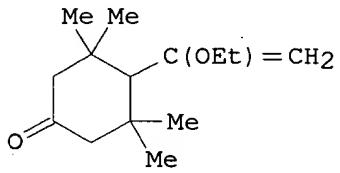
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3953516	A	19760427	US 1975-546533	19750203
US 3578715	A	19710511	US 1966-585259	19661010
US 3875241	A	19750401	US 1971-110652	19710128
US 3953471	A	19760427	US 1975-546532	19750203

PRIORITY APPLN. INFO.:
CH 1965-14216 19651014
US 1966-585259 19661010
US 1971-110652 19710128

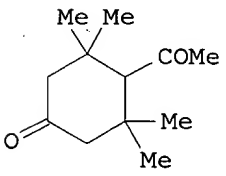
GRAPHIC IMAGE:



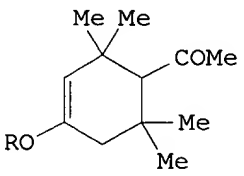
I



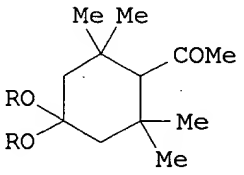
II



III



IV



V

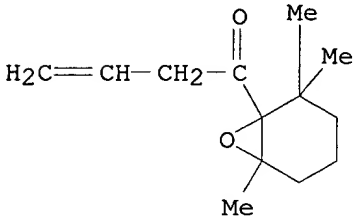
ABSTRACT:
Concurrent cyclodimerization of Me2C:CHCOMe and its reaction with HC(OEt)3 in the presence of BF3.Et2O gave a mixt. of I and II which was hydrolyzed to III. III with HC(OR)3 (R = Et, Pr, Bu, Me2CHCH2, amyl, isoamyl) in the presence of BF3.Et2O gave IV and V. The enol ethers and ketals are useful in ***perfumes*** .

L6 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN

IT **31089-87-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and isomerization of)

RN 31089-87-9 CAPLUS

CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)

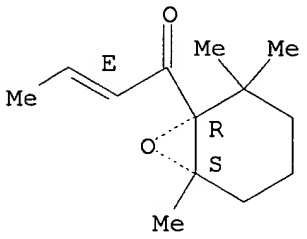


IT **31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 31191-88-5 CAPLUS

CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

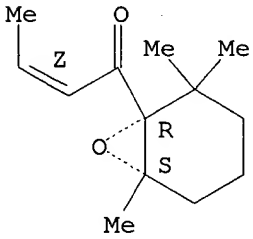
Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS

CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1976:446082 CAPLUS
DOCUMENT NUMBER: 85:46082
TITLE: Cycloaliphatic unsaturated ketones as **odor**- and taste-modifying agents

INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich S. A., Switz.
SOURCE: U.S., 34 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

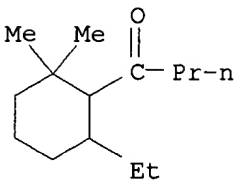
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3928456	A	19751223	US 1974-503794	19740906
CH 498795	A	19701115	CH 1968-498795	19681101
CH 537452	A	19730713	CH 1969-12065	19690808
ES 377485	A1	19720701	ES 1970-377485	19700313
ES 377483	A1	19720701	ES 1970-377483	19700313
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
DD 96077	W	19730312	DD 1970-153631	19700507
US 3975310	A	19760817	US 1974-503738	19740906
US 3931326	A	19760106	US 1974-523743	19741114
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

PRIORITY APPLN. INFO.:

CH 1967-15667	19671109
CH 1968-16309	19681101
US 1968-774179	19681107
CH 1969-6976	19690507
CH 1969-12065	19690808
CH 1970-5559	19700414
CH 1970-5725	19700417
US 1970-35594	19700507
CH 1970-6725	19700417
US 1974-503738	19740906
US 1976-676505	19760413

ABSTRACT:
Polymethyl (unsatd. acyl) cyclohexenes and -cyclohexadienes and polymethylbicyclo[4.3.0]nona-2,8-dien-7-ones and -non-8-en-7-ones were prepd.; the first 2 types of ketones were useful in floral **perfumes** and all 4 ketone groups were useful as flavoring agents for foods and beverages (compns. given). Thus, 1-(1-hydroxy-3-butenyl)-2,6,6-trimethylcyclohexene was oxidized by Cr2O3 to 1-(3-butenoyl)-2,6,6-trimethylcyclohexene, and this was isomerized by p-MeC6H4SO3H in benzene to trans-1-crotonoyl-2,6,6-trimethylcyclohexene, which increased the power and richness of floral **perfumes** and was used in tutti-frutti flavoring compns., in flavor compns. for monastery type liquor, and in a soln. which increased the aromaticity of black tea.

L6 ANSWER 19 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **57935-16-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 57935-16-7 CAPLUS
CN 1-Butanone, 1-(6-ethyl-2,2-dimethylcyclohexyl)- (9CI) (CA INDEX NAME)



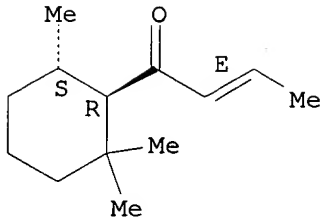
ACCESSION NUMBER: 1976:44470 CAPLUS
DOCUMENT NUMBER: 84:44470
TITLE: Cycloaliphatic unsaturated ketones as flavors and **perfumes**
PATENT ASSIGNEE(S): Naarden International N. V., Neth.
SOURCE: Ger. Offen., 39 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2508060	A1	19750904	DE 1975-2508060	19750221
GB 1456151	A	19761117	GB 1974-8165	19740222
BE 825840	A2	19750821	BE 1975-153616	19750221
NL 7502123	A	19750826	NL 1975-2123	19750221
JP 50117961	A2	19750916	JP 1975-21084	19750221
FR 2262012	A1	19750919	FR 1975-5555	19750221
FR 2262012	B1	19800418		
ES 434932	A1	19761216	ES 1975-434932	19750221
CH 612846	A	19790831	CH 1975-2177	19750221
CA 1097689	A1	19810317	CA 1975-220558	19750221

PRIORITY APPLN. INFO.: GB 1974-8165 19740222
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Thirty-three alicyclic unsatd. ketones (I-VII R = Et, Pr, R1 = CH:CHMe, Pr, C.tplbond.CMe, Z = CHMe, CHEt), were prepd. by treating the appropriate cyclohexanecarboxylate deriv. with alkyllithium and optional hydrogenation. E.g., 41 g Et 2-ethyl-6,6-dimethyl-2-cyclohexenecarboxylate was treated with CH2:CHCH2Li soln. (prepd. from 12.5 g Li and 80 g CH2:CHCH2OPh in THF-ether) at -75.degree. to give 24 g a mixt. contg. 50% I (R = Et, R1 = CH:CHMe), 10% II, and 25% III (Z = CHMe). I-VII were useful in **perfume** compositions.

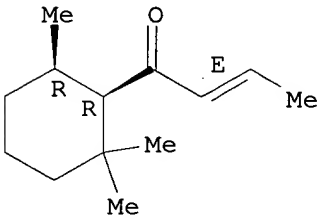
L6 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **52842-35-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(flavoring material and **perfume**, prepn. of)
RN 52842-35-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.beta.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



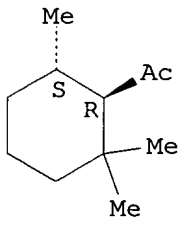
IT **52842-32-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(**perfume**, prepn. of)
RN 52842-32-7 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.alpha.]-(9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



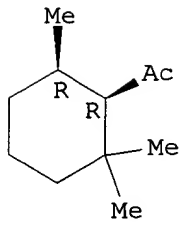
IT **52842-33-8P 52842-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation reaction with acetaldehyde)
RN 52842-33-8 CAPLUS
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

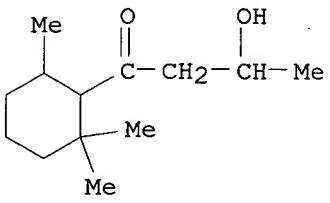


RN 52842-34-9 CAPLUS
CN Ethanone, 1-[(1R,6R)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

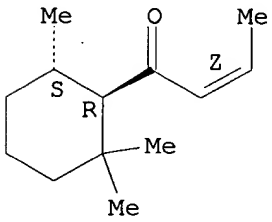


IT **39900-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydration of)
RN 39900-17-9 CAPLUS
CN 1-Butanone, 3-hydroxy-1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



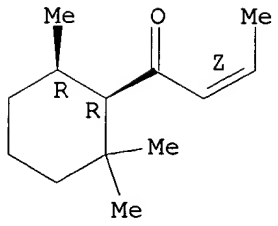
IT **52842-37-2P 56782-86-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 52842-37-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 56782-86-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.alpha.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1975:478718 CAPLUS
DOCUMENT NUMBER: 83:78718
TITLE: Crotonoyltrimethylcyclohexane **perfumes** and flavoring materials
INVENTOR(S): De Haan, Douwe R.; Kettenes, Dirk K.
PATENT ASSIGNEE(S): Beheer, P. F. W., B. V., Neth.
SOURCE: Brit., 7 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

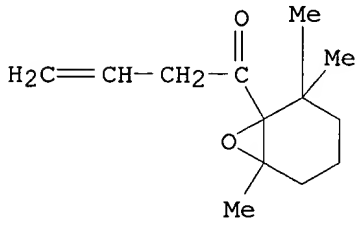
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1390654	A	19750416	GB 1972-49368	19731024
NL 7314428	A	19740501	NL 1973-14428	19731019
NL 177826	B	19850701		
NL 177826	C	19851202		
CA 1020582	A1	19771108	CA 1973-183974	19731023
BE 806536	A2	19740425	BE 1973-7000466	19731025
DE 2353578	A1	19740509	DE 1973-2353578	19731025
DE 2353578	C2	19850905		
AU 7361849	A1	19750501	AU 1973-61849	19731025
FR 2204625	A1	19740524	FR 1973-38245	19731026
JP 50052046	A2	19750509	JP 1973-120623	19731026
JP 57036252	B4	19820803		
IT 1003200	A	19760610	IT 1973-30634	19731026
CH 585049	A	19770228	CH 1973-15092	19731026
US 4109022	A	19780822	US 1976-681202	19760428
US 4136066	A	19790123	US 1978-896224	19780413

PRIORITY APPLN. INFO.:
GB 1972-49368 19721026
US 1973-409099 19731024
US 1976-681202 19760428

ABSTRACT:
Trans,E-1-crotonoyl-2,2,6-trimethylcyclohexane (I), of a strong fresh fruity ***odor*** devoid of woody and .beta.-ionone character, was prepd. from cis-1-acetyl-2,2,6-trimethylcyclohexane by successive epimerization, condensation with MeCHO, and dehydration. I improved the flavor of raspberry and rhubarb flavoring compns. and of red currant juice conc. The cis,E-isomer (II), of a predominantly earthy-minty **odor**, was prepd. from cis-1-acetyl-2,2,6-trimethyl-4-cyclohexene by successive hydrogenation, condensation with MeCHO, and dehydration. The trans,Z-isomer (III) was prepd. from trans-dihydroionone by successive epoxidn., Wharton reaction, and oxidn. A 9:60:4:27 mixt. of I, II, III, and the cis,Z-isomer was prepd. from .alpha.-ionone by successive epoxidn., hydrogenation, Wharton reaction, and oxidn.

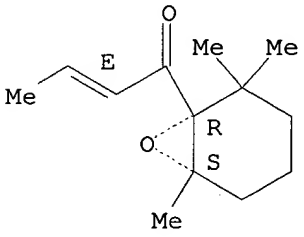
L6 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31089-87-9P 31191-88-5P 35122-44-2P**
RL: PREP (Preparation)

(prepn. and use in **perfume** compns.)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)

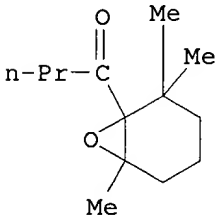


RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 35122-44-2 CAPLUS
CN 1-Butanone, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1975:160116 CAPLUS
DOCUMENT NUMBER: 82:160116
TITLE: Use of alicyclic oxygenated compounds as **perfume** agents
INVENTOR(S): Schulte-Elte, Karl H.
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Patentschrift (Switz.), 9 pp. Division of Swiss 548,967 (CA 81: 77558t).
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

CH 557422	A	19741231	CH 1972-16032	19710913
PRIORITY APPLN. INFO.:			CH 1972-16032	19710913

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

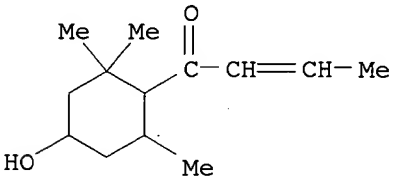
ABSTRACT:
I and II are prepd. and used in **perfume** compns. wherein R = CH(OH)CHn...CH...CH4-n (n = 1 or 2), CH(OH)Pr or COCH:CHCMe3, Y = CH(OAc)CHn...CH...CH4-n (n = 1 or 2), CH(OAc)Pr, COPr, and Z = pi bond or O. I were prepd. by the oxidn. of appropriate 1-cyclohexenes with singlet state O followed by treatment of the oxidn. product with a reducing agent. For example, a mixt. of 2,6,6-trimethyl-1-(1-hydroxy-2-butenyl)cyclohex-1-ene (III) [35124-05-1] (20.5 g), Rose Bengal (0.2 g), and NaOAc (1 g) in MeOH (160 ml) traversed by a stream of O was irradiated at 15.degree. with a Hg vapor lamp for 6 hr, and the resulting soln. (95 ml) was treated with a soln. of Na2SO3 (5 g) in 200 ml H2O first at 0-5.degree. and then at 40.degree. for 2 hr, and worked up to give by prep. gas chromatog. the following I (R = CH(OH)CH:CHMe, 2-substituent, stereoisomer, and % yield given): :CH2, threo, 30, (IV); :CH2, erythro, 6, (V); Me, -, 4 (VI). Also obtained was 48% trans-2,6,6-trimethyl-1-(2-butenoyl)-1,2-epoxycyclohexane [**31191-88-5**]. I with a 2-methylene group were also prepd. by treating appropriate epoxides with a basic agent. For example, a suspension of III (19.4 g) and NaOAc (12 g) in CH2Cl2 (35 ml) was treated with 40% aq. AcOOH (21 g) and NaOAc (0.6 g) at 20.degree. under a stream of N for 2 hr, and worked up to give the corresponding 1,2-epoxycyclohexane, (VII), b.0 4 84.degree.. VII (10.5 g) was treated with 50 ml of 1N soln. of Li in NH2CH2CH2NH2 and worked up to give in 22% yield a mixt. of IV and V. I (X = COCH:CHMe, 2-Me) was prepd. by oxidn. of VI with MnO2. CrO3/pyridine is an alternate oxidizing agent. II were prepd. from cyclohex-1-enes bearing appropriate hydroxyl-substituted Y groups by acetylation followed by epoxidation. For example, III was acetylated with AcCl/PhNMe2 to give II (Z = pi bond, Y = CH(OAc)CH:CHMe), (VIII), b.0 1 62.degree.. VIII was subjected to epoxidation and the product was sepd. by prep. gas chromatog. to give pure diastereoisomers of II (Z = O, Y = CH(OAc)CH:CHMe, threo 52%, erythro 47%). **Perfume** compns. incorporating the compds. were given.

L6 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN

IT **53398-17-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of)

RN 53398-17-7 CAPLUS

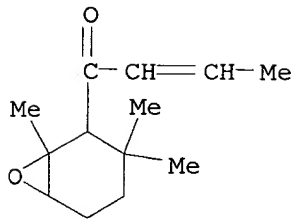
CN 2-Buten-1-one, 1-(4-hydroxy-2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



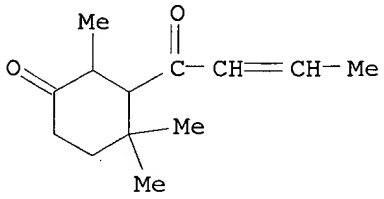
IT **43052-86-4P 53398-06-4P 53398-07-5P**
53398-15-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 43052-86-4 CAPLUS

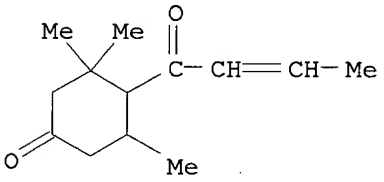
CN 2-Buten-1-one, 1-(1,3,3-trimethyl-7-oxabicyclo[4.1.0]hept-2-yl)- (9CI) (CA INDEX NAME)



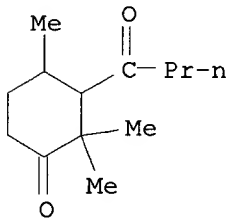
RN 53398-06-4 CAPLUS
CN Cyclohexanone, 2,4,4-trimethyl-3-(1-oxo-2-butenyl)- (9CI) (CA INDEX NAME)



RN 53398-07-5 CAPLUS
CN Cyclohexanone, 3,3,5-trimethyl-4-(1-oxo-2-butenyl)- (9CI) (CA INDEX NAME)



RN 53398-15-5 CAPLUS
CN Cyclohexanone, 2,2,4-trimethyl-3-(1-oxobutyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1974:491132 CAPLUS
DOCUMENT NUMBER: 81:91132
TITLE: Oxygen-containing cycloaliphatic compounds
INVENTOR(S): Schulte-Elte, Karl H.; Jindra, Henri
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Ger. Offen., 43 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

DE 2353468	A1	19740509	DE 1973-2353468	19731025
CH 571565	A	19760115	CH 1972-15691	19721026
CH 566135	A	19750915	CH 1973-4096	19730321
US 3927107	A	19751216	US 1973-408919	19731023
GB 1386060	A	19750305	GB 1973-49983	19731026
US 3957877	A	19760518	US 1975-560225	19750320

PRIORITY APPLN. INFO.: CH 1972-15691 19721026
CH 1973-4096 19730321
US 1973-408919 19731023

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

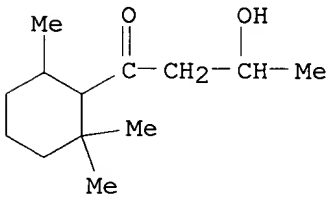
ABSTRACT:
Cyclohexanones and cyclo-hexenones, e.g., I, II, III, and IV, were useful as ***perfumes*** and flavoring materials. Oxidn. of V with Na2Cr2O7 in Ac2Ogave III and oxidn. of VI with Se oxide and dioxane gave IV. About 10 compds. were prepd.

L6 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN

IT **39900-17-9P 52842-32-7P 52842-33-8P**
52842-34-9P 52842-35-0P 52842-37-2P
52843-92-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 39900-17-9 CAPLUS

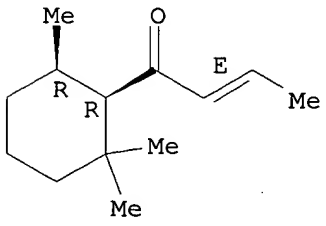
CN 1-Butanone, 3-hydroxy-1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 52842-32-7 CAPLUS

CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.alpha.]- (9CI) (CA INDEX NAME)

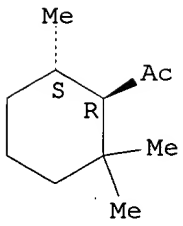
Relative stereochemistry.
Double bond geometry as shown.



RN 52842-33-8 CAPLUS

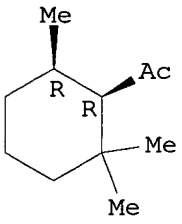
CN Ethanone, 1-[(1R,6S)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



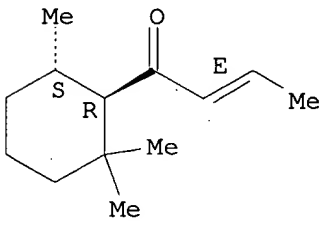
RN 52842-34-9 CAPLUS
CN Ethanone, 1-[(1R,6R)-2,2,6-trimethylcyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



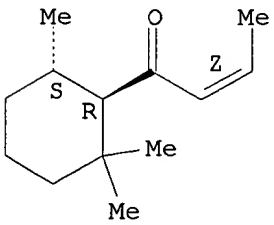
RN 52842-35-0 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(E),6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



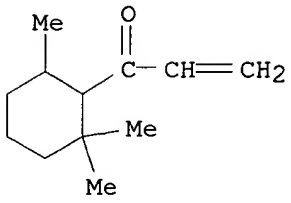
RN 52842-37-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.beta.]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 52843-92-2 CAPLUS
CN 2-Propen-1-one, 1-(2,2,6-trimethylcyclohexyl)-, [1.alpha.(Z),6.alpha.]-

(9CI) (CA INDEX NAME)

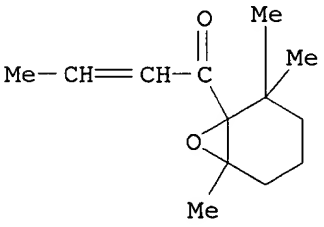


ACCESSION NUMBER: 1974:425196 CAPLUS
DOCUMENT NUMBER: 81:25196
TITLE: Stereoisomers of 1-crotonyl-2,2,6-trimethylcyclohexane for use in **perfumes**
INVENTOR(S): De Haan, Douwe R.; Kettenes, Dirk K.
PATENT ASSIGNEE(S): P.F.W. Beheer B. V.
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2353578	A1	19740509	DE 1973-2353578	19731025
DE 2353578	C2	19850905		
GB 1390654	A	19750416	GB 1972-49368	19731024

PRIORITY APPLN. INFO.: GB 1972-49368 19721026
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The four stereoisomers of 1-crotonyl-2,2,6-tri-methylcyclohexane (I, II, III, IV), useful as **perfume** ingredients, were prepd. by the epoxidn. of .alpha.-ionone, followed by hydrogenation over Pt to give a mixt. of epoxides, which, after reaction with N2H4 in AcOH and oxidn. with MnO2, gave a mixt. of I, II, III, and IV.

L6 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **51200-85-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acids)
RN 51200-85-2 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



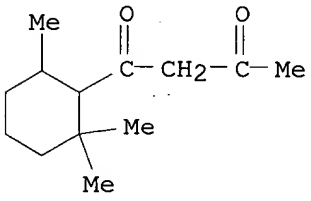
ACCESSION NUMBER: 1974:74276 CAPLUS
DOCUMENT NUMBER: 80:74276
TITLE: Utilization of hydroxylated compounds as **perfuming** agents

INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Patentschrift (Switz.), 3 pp. Division of Swiss 528,470 (Ger. 2,022,216, (CA 74;76564k).
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 539682	A	19730914	CH 1972-12363	19700414

PRIORITY APPLN. INFO.: CH 1972-12363 19700414
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
The title materials, such as 2,6,6-trimethyl-1-hydroxy-1-(2-butyryl)-2-cyclohexene (I), are prepd. and used at 0.1-1 wt.% of a **perfume** mixt. to improve the strength, diffusion, and richness of the **perfume**, and to give it a spicy note. I, b0.01 80.degree., is prepd. by treating cis- and trans-2,6,6-trimethyl-1-(2-butyryl)-1,2-epoxycyclohexane with an acid such as clayey earth, HCl, H3PO4, or H2SO4.

L6 ANSWER 25 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **39900-14-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 39900-14-6 CAPLUS
CN 1,3-Butanedione, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1974:59575 CAPLUS
DOCUMENT NUMBER: 80:59575
TITLE: Alicyclic ketones
INVENTOR(S): Schulte-Elte, Karl H.
PATENT ASSIGNEE(S): Firmenich S. A.
SOURCE: Ger. Offen., 43 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2315640	A1	19731011	DE 1973-2315640	19730329
DE 2315640	B2	19791115		
DE 2315640	C3	19800724		
CH 561676	A	19750515	CH 1972-4770	19720330
NL 7304365	A	19731002	NL 1973-4365	19730329
FR 2178221	A1	19731109	FR 1973-11446	19730329
JP 49007250	A2	19740122	JP 1973-36558	19730330

JP 53046834	B4	19781216			
GB 1391736	A	19750423	GB 1973-15562	19730330	
US 3923896	A	19751202	US 1973-346296	19730330	
US 3968161	A	19760706	US 1975-598132	19750722	

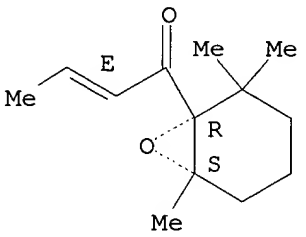
PRIORITY APPLN. INFO.:
CH 1972-4770 19720330
US 1973-346296 19730330

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

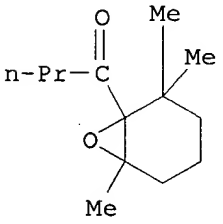
ABSTRACT:
Unsatd. ketones (I) (R, R1, R3, R4, R5 = H, alkyl; R2 = :CH2, Me; n = 0, 1; X = O, OH, NH, NH2) with double bonds in the 1-, 2-, 3-, or 4-position of the ring, conjugated in the 1,3-positions of the ring, in the 2- or 3-position of the side chain, or in both the ring and side chain, were prepd. by various schemes based on reactions of .alpha.- (II), .beta.-, or .gamma.-ionone derivs. or damascenone (III) derivs. Several I were tested in **perfume** compns. and as flavorants.

L6 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31191-88-5P 35122-44-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 35122-44-2 CAPLUS
CN 1-Butanone, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1973:442041 CAPLUS
DOCUMENT NUMBER: 79:42041
TITLE: Oxygenated cycloaliphatics
INVENTOR(S): Schulte-Elte, Karl Heinrich
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 46 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2244680	A1	19730322	DE 1972-2244680	19720912
DE 2244680	C2	19821028		
CH 548967	A	19740515	CH 1971-13397	19710913

PRIORITY APPLN. INFO.: CH 1971-13397 19710913

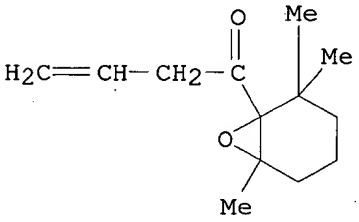
ABSTRACT:
The prepn. of a variety of cyclohexane derivs. (I-IV) with a fruity ***odor*** , useful as **perfumes** or in flavorings, was given. Thus, III (R = CHOHCH:CHMe) was oxidized by pure O, then reduced by Na2SO3 to give 48 trans-IV (R2 = COCH:CHMe), 30 threo- and 6 erythro-I [R2 = CH(OH)CH:CHMe, R1 = H], and 4% II (R and R1 same as in I).

L6 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN

IT **31089-87-9P 31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 31089-87-9 CAPLUS

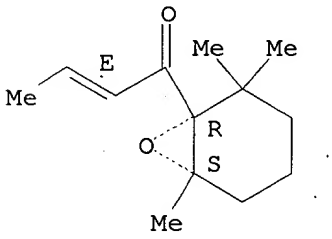
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



RN 31191-88-5 CAPLUS

CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

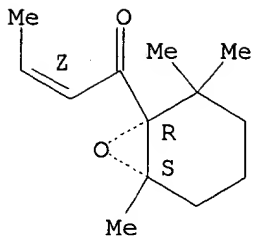
Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS

CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1973:431582 CAPLUS
DOCUMENT NUMBER: 79:31582
TITLE: Cycloaliphatic unsaturated alcohols
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 108 pp. Division of Ger. Offen. 2,022,216 (CA 74;76564k).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

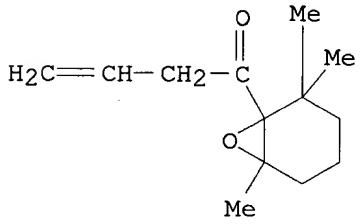
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2065323	A1	19730322	DE 1970-2065323	19700506
CH 537452	A	19730713	CH 1969-12065	19690808
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
NL 7006649	A	19701110	NL 1970-6649	19700506
NL 163211	B	19800317		
NL 163211	C	19800815		
GB 1305621	A	19730207	GB 1970-22215	19700507
DD 96077	W	19730312	DD 1970-153631	19700507
JP 55003328	B4	19800124	JP 1970-38587	19700507
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

PRIORITY APPLN. INFO.:
CH 1969-6976 19690507
CH 1969-12065 19690808
CH 1970-5559 19700414
CH 1970-5725 19700417
CH 1967-15667 19671109
CH 1968-16309 19681101
US 1968-774179 19681107
CH 1970-6725 19700417
US 1970-35594 19700507
US 1974-503738 19740906
US 1976-676505 19760413

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Ethylenic cyclohexanemethanol derivs. with unsatn. in the ring, in an .alpha.-alkenyl group or a 2-methylene group, or in a combination of these were prepd., e.g., by reaction of a cyclocitral with an alkenyllithium compd. The products, esp. intermediate ketones, were intensely arom. and formulations were given for their use in **perfumes** and as flavoring materials for liqueurs and foods. Among the title compds. and arom. ketone intermediates prepd. were I-III.

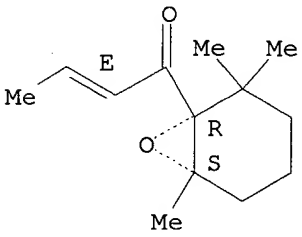
L6 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN

IT **31089-87-9P 31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



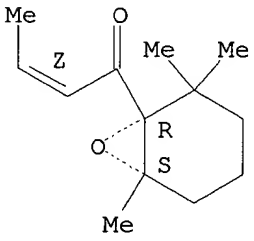
RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER:	1973:418208 CAPLUS
DOCUMENT NUMBER:	79:18208
TITLE:	Cycloaliphatically unsaturated epoxy compounds
INVENTOR(S):	Kovats, Erwin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S):	Firmenich et Cie.
SOURCE:	Ger. Offen., 108 pp. Division of Ger. Offen. 2,022,216 (CA 74;76564k). CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German

FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

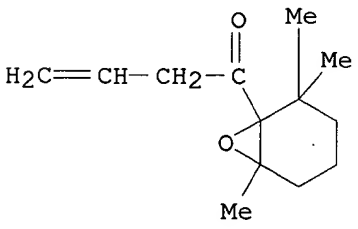
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2065322	A1	19730329	DE 1970-2065322	19700506
DE 2065322	B2	19790719		
DE 2065322	C3	19800320		
CH 537452	A	19730713	CH 1969-12065	19690808
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
NL 7006649	A	19701110	NL 1970-6649	19700506
NL 163211	B	19800317		
NL 163211	C	19800815		
GB 1305621	A	19730207	GB 1970-22215	19700507
DD 96077	W	19730312	DD 1970-153631	19700507
JP 55003328	B4	19800124	JP 1970-38587	19700507
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

PRIORITY APPLN. INFO.:

CH 1969-6976	19690507
CH 1969-12065	19690808
CH 1970-5559	19700414
CH 1970-5725	19700417
CH 1967-15667	19671109
CH 1968-16309	19681101
US 1968-774179	19681107
CH 1970-6725	19700417
US 1970-35594	19700507
US 1974-503738	19740906
US 1976-676505	19760413

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Epoxycyclohexanes I were prepd. by epoxidn. of the corresponding cyclohexenes. Prepn. of the starting alcs. and ketones was given; both the unepoxidized and epoxidized ketones had a pleasant **odor**, usually fruity, and formulations were given for their use in **perfume** and as flavoring materials for liqueurs and foods.

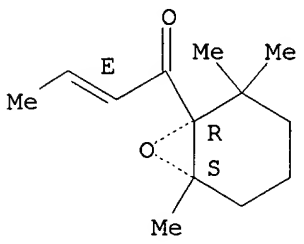
L6 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31089-87-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(isomerization of)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



IT **31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31191-88-5 CAPLUS

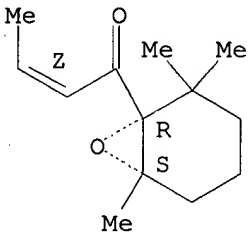
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)-
(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)-
(8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



ACCESSION NUMBER: 1973:418207 CAPLUS
DOCUMENT NUMBER: 79:18207
TITLE: Cycloaliphatically unsaturated ketones
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Ohloff, Guenther; Stoll, Max
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 108 pp. Division of Ger. Offen. 2,022,216 (CA 74;76565k).
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

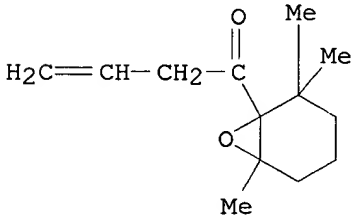
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2065324	A1	19730329	DE 1970-2065324	19700506
DE 2065324	B2	19790726		
DE 2065324	C3	19800403		
CH 537452	A	19730713	CH 1969-12065	19690808
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
NL 7006649	A	19701110	NL 1970-6649	19700506
NL 163211	B	19800317		
NL 163211	C	19800815		
GB 1305621	A	19730207	GB 1970-22215	19700507
DD 96077	W	19730312	DD 1970-153631	19700507
JP 55003328	B4	19800124	JP 1970-38587	19700507
US 4187863	A	19800212	US 1977-782536	19770329

US 4226892 A 19801007 US 1978-900522 19780427
PRIORITY APPLN. INFO.: CH 1969-6976 19690507
CH 1969-12065 19690808
CH 1970-5559 19700414
CH 1970-5725 19700417
CH 1967-15667 19671109
CH 1968-16309 19681101
US 1968-774179 19681107
CH 1970-6725 19700417
US 1970-35594 19700507
US 1974-503738 19740906
US 1976-676505 19760413

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

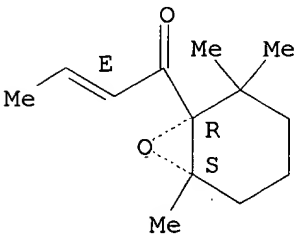
ABSTRACT:
MeCH:CMeCH2CHMeCH:CMeCHO was cyclized to 2,4,6,6-tetramethyl-1-cyclohexene-1-carboxaldehyde, which was treated with MeCH:CH2Li to give an alc., which was oxidized to the ketone I. Approx. 20 other ethylenic cyclohexyl ketones were prepd. similarly; these compds. had a pleasant **odor**, usually fruity, and formulations were given for their use in **perfumes** and as flavoring materials for liqueurs and foods.

L6 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **31089-87-9P 31191-88-5P 31191-89-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31089-87-9 CAPLUS
CN 3-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)- (8CI, 9CI) (CA INDEX NAME)



RN 31191-88-5 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (E)- (8CI, 9CI) (CA INDEX NAME)

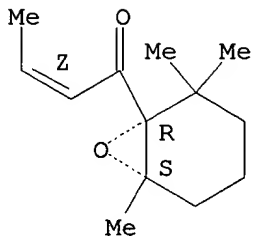
Relative stereochemistry.
Double bond geometry as shown.



RN 31191-89-6 CAPLUS
CN 2-Buten-1-one, 1-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-, (Z)- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



ACCESSION NUMBER: 1971:76564 CAPLUS
DOCUMENT NUMBER: 74:76564
TITLE: Cycloaliphatic unsaturated ketones for use as **perfumes**
INVENTOR(S): Kovats, Ervin; Demole, Edouard; Stoll, Max; Ohloff, Guenther
PATENT ASSIGNEE(S): Firmenich et Cie.
SOURCE: Ger. Offen., 137 pp. Addn. to Ger. Offen. 1,807,568
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2022216	A	19701119	DE 1970-2022216	19700506
DE 2022216	B2	19760701		
DE 2022216	C3	19770217		
CH 537452	A	19730713	CH 1969-12065	19690808
CH 528470	A	19720930	CH 1970-528470	19700414
CH 529709	A	19721031	CH 1970-529709	19700417
BE 750049	A	19701106	BE 1970-750049	19700506
NL 7006649	A	19701110	NL 1970-6649	19700506
NL 163211	B	19800317		
NL 163211	C	19800815		
GB 1305621	A	19730207	GB 1970-22215	19700507
DD 96077	W	19730312	DD 1970-153631	19700507
JP 55003328	B4	19800124	JP 1970-38587	19700507
US 4187863	A	19800212	US 1977-782536	19770329
US 4226892	A	19801007	US 1978-900522	19780427

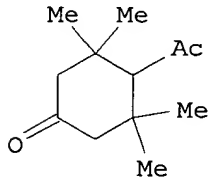
PRIORITY APPLN. INFO.:

CH 1969-6976	19690507
CH 1969-12065	19690808
CH 1970-5559	19700414
CH 1970-5725	19700417
CH 1967-15667	19671109
CH 1968-16309	19681101
US 1968-774179	19681107
CH 1970-6725	19700417
US 1970-35594	19700507
US 1974-503738	19740906
US 1976-676505	19760413

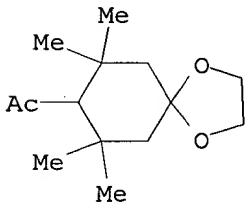
ABSTRACT:
Stereoisomers of cyclic unsatd. ketones (I-V, R, R1, R2, R3 = H or Me) were prepd. A mixt. of MeCH:CMeCH2CHMeCH:CMeCHO and MeCH:CMeCH2CMe2CH:CHCHO was treated with PhNH2-Na2SO4 in Et2O to give a 4-methyl-.alpha. and 4-methyl-.beta.-cyclocitral mixt., which was treated with alc. KOH to give 4-methyl-.beta.-cyclocitral (VI). VI was treated with MeCH:CHLi to give 2,4,6,6-tetramethyl-1-(1-hydroxy-2-butenyl)-1-cyclohexene, which was oxidized with MnO2 to give 2,4,6,6-tetramethyl-1-trans-crotonoyl-1-cyclohexene (I, R = R1 = R3 = H, R2 = Me) (VII). Dehydrogenation of VII with N-bromosuccinimide-

azodiisobutyronitrile in CH2Cl2 gave 2,4,6,6-tetramethyl-1-trans-crotonoyl-1,3-hexadiene (II, R = R1 = R3 = H, R2 = Me): .apprx.11 I-II were also prepd. 2,6,6-Trimethyl-1-(1-hydroxy-3-butenyl)-1-cyclohexene was epoxidized with Ac-O2H-NaOAc to give 2,6,6-trimethyl-1-(1-hydroxy-3-butenyl)-1,2-epoxycyclohexane, which was oxidized with Na2Cr2O7 (to give the corresponding ketone), followed by treatment with NaOAc in dioxane, to give cis- and trans-2,6,6-trimethyl-1-crotonoyl-1,2-epoxycyclohexane (III, R = R1 = R2 = R3 = H). Treatment of the cis-trans-epoxycyclohexane mixt. with acidc kieselguhr in dioxane gave 2,6,6-trimethyl-1-hydroxy-1-crotonyl-2-cyclohexane. Cyclization of 2,6,6-trimethyl-1-(2-methylcrotonoyl)-1-cyclohexene (I, R = R2 = R3 = H, R1 = Me) with acidic kieselguhr in dioxane gave 1,5,5,8,9-pentamethylbicyclo-[4.3.0] non-8-en-7-one (IV, R = H, R1 = Me). Cyclization of 2,6,6-trimethyl-1-crotonoyl-2-cyclohexene in the presence of BF3 in benzene gave 4,4,8-trimethyl-9-methylenebicyclo [3.3.1]-non-6-ene (V).

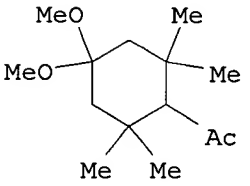
L6 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **16556-46-0P 16556-47-1P 16556-49-3P**
16556-57-3P 16556-58-4P 16556-59-5P
16556-60-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16556-46-0 CAPLUS
CN Cyclohexanone, 4-acetyl-3,3,5,5-tetramethyl- (8CI, 9CI) (CA INDEX NAME)



RN 16556-47-1 CAPLUS
CN Ethanone, 1-(7,7,9,9-tetramethyl-1,4-dioxaspiro[4.5]dec-8-yl)- (9CI) (CA INDEX NAME)

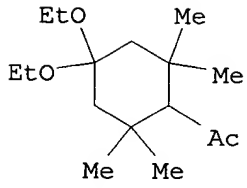


RN 16556-49-3 CAPLUS
CN Ethanone, 1-(4,4-dimethoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)

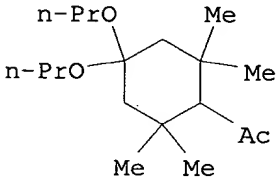


RN 16556-57-3 CAPLUS
CN Ethanone, 1-(4,4-diethoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX

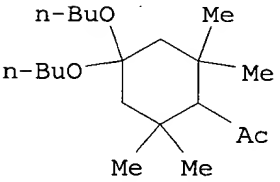
NAME)



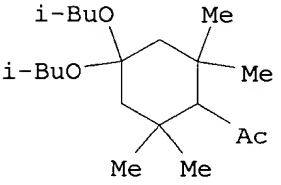
RN 16556-58-4 CAPLUS
CN Ethanone, 1-(2,2,6,6-tetramethyl-4,4-dipropoxycyclohexyl)- (9CI) (CA INDEX NAME)



RN 16556-59-5 CAPLUS
CN Ethanone, 1-(4,4-dibutoxy-2,2,6,6-tetramethylcyclohexyl)- (9CI) (CA INDEX NAME)



RN 16556-60-8 CAPLUS
CN Ethanone, 1-[2,2,6,6-tetramethyl-4,4-bis(2-methylpropoxy)cyclohexyl]- (9CI) (CA INDEX NAME)



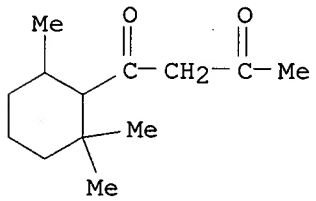
ACCESSION NUMBER: 1967:481846 CAPLUS
DOCUMENT NUMBER: 67:81846
TITLE: 4-Acetyl-3,3,5,5-tetramethylcyclohexanones
PATENT ASSIGNEE(S): Etablissements Roure-Bertrand Fils and Justin Dupont
SOURCE: Neth. Appl., 12 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

NL 6614506	A	19670417	NL 1966-14506	19661014
BE 687954	A	19670407	BE 1966-687954	19661007
SE 352619	B	19730108	SE 1966-13968	19661014
DK 136191	B	19770829	DK 1966-5329	19661014

PRIORITY APPLN. INFO.: CH 1965-14216 19651014
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
ABSTRACT:
Title compds. (e.g., I), are prepd. by treating mesityl oxide (II) with a low alkyl orthoformate and hydrolyzing the enol ethers formed. Thus, 1 mole ethyl orthoformate (III) was added to 4 moles II and 1 cc. BF3 etherate during 4 hrs. at 50.degree.. The temp. was kept at 50.degree. an addnl. 4 hrs., after which 5 g. powd. Na2CO3 was added and the mixt. stirred 30 min. After rectification 70 g. of a mixt., b. 75-84.degree., was obtained from which 4-(1-ethoxyvinyl)-3,3,5,5-tetramethylcyclohexanone (IV), b2 80-2.degree., n15D 1.4758, carbonyl index 245, was isolated. The above expt. was repeated using 1.2 moles II and 1 mole III to yield IV and 1-ethoxy-4-(1-ethoxyvinyl)-3,3,5,5-tetramethyl-1-cyclohexene, b2 74-6.degree., n15D 1.4744, carbonyl index 220. Hydrolysis of the above formed compds. gave I, b2 108.degree., n15D 1.4786. The following compds. were similarly prepd.: 4-(1-methoxyvinyl)-3,3,5,5-tetramethylcyclohexanone, b1 90-2.degree., m. 45.degree., and 1-methoxy-4-(1-methoxyvinyl)-3,3,5,5-tetramethyl-1-cyclohexene, b1 82-4.degree., n15D 1.4872; a mixt. of the corresponding propyl enol ethers, b1 95-100.degree., n15D 1.4795; a mixt. of the corresponding isobutyl enol ethers, b1 110-20.degree., n15D 1.4775; a mixt. of the corresponding isoamyl enol ethers, b1 110-20.degree., n15D 1.4780. The following I were also prepd.: 4-acetyl-1,1-ethylenedioxy-3,3,5,5-tetramethylcyclohexane, m. 113.0-13.5.degree.; 4-acetyl-1-methoxy-3,3,5,5-tetramethyl-1-cyclohexene, b1 78-80.degree., n15D 1.4780; 4-acetyl-1,1-dimethoxy-3,3,5,5-tetramethylcyclohexane, b1 90-3.degree., m. 59-60.degree.; 4-acetyl-1-ethoxy-3,3,5,5-tetramethyl-1-cyclohexene, b1 90.degree., nD15 1.4745; 4-acetyl-1-propoxy-3,3,5,5-tetramethyl-1-cyclohexene, b0.4 92.degree., n15D 1.4749; 4-acetyl-1-butoxy-3,3,5,5,-tetramethyl-1-cyclohexene, b0.4 97-9.degree., n15D 1.4735; 4-acetyl-1-isobutoxy-3,3,5,5-tetramethyl-1-cyclohexene, b0.5 107-9.degree., n15D 1.4712; 4-acetyl-1-n-amyloxy-3,3,5,5-tetramethyl-1-cyclohexene, b0.3 101-4.degree., n15D 1.4630; 4-acetyl-1-isoamyloxy-3,3,5,5-tetramethyl-1-cyclohexene, b0.2 106-8.degree., n15D 1.4658; 4-acetyl-1-allyloxy-3,3,5,5-tetramethyl-1-cyclohexene, b0.5 95-100.degree., n15D 1.4846; 4-acetyl-1,1-diethoxy-3,3,5,5-tetramethylcyclohexane, b1 104.degree., n15D 1.4676; 4-acetyl-1,1-dipropoxy-3,3,5,5-tetramethylcyclohexane, b0.4 118.degree., n15D 1.4676; 4-acetyl-1,1-diisobutoxy-3,3,5,5-tetramethylcyclohexane, b0.5 125-8.degree., m. 48.degree.; 1-acetoxy-4-acetyl-3,3,5,5-tetramethyl-1-cyclohexene, m. 92-4.degree./0.3 mm., n15D 1.cntdot.4785. I and its derivs. are useful as ***scents*** .

L6 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2003 ACS on STN
IT **39900-14-6**, 1,3-Butanedione, 1-(2,2,6-trimethylcyclohexyl)-
(prepn. of)
RN 39900-14-6 CAPLUS
CN 1,3-Butanedione, 1-(2,2,6-trimethylcyclohexyl)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1949:25971 CAPLUS

DOCUMENT NUMBER: 43:25971
ORIGINAL REFERENCE NO.: 43:4813c-i,4814a
TITLE: Violet **perfumes**. XXVIII. Ketotetrahydroionone
AUTHOR(S): Prelog, V.; Frick, H.
SOURCE: Helvetica Chimica Acta (1948), 31, 2135-42
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
ABSTRACT:

cf. C.A. 43, 3798d. In an unsuccessful effort to determine the structure of the tetrahydroionone deriv. (I), contg. an addnl. O function, which was isolated from pregnant mare's urine (C.A. 43, 3798f), .alpha.'-, .beta.'-, and 4-ketotetrahydroionones were prepd. cis-Tetrahydroionone (1.0 g.) in 4 cc. abs. alc. with 4 drops concd. H_2SO_4 was decompd. at 45.degree. with 1.1 g. n-$BuNO_2$ heated 2 hrs. at 45.degree., taken up in Et_2O, extd. with 10% NaOH, and the alk. ext. acidified to give 0.45 g. of the .alpha.'-iso-nitroso deriv.; steam distn. from 4 g. $(COOH)_2$ gave 0.25 g. .alpha.'-keto-cis-tetrahydroionone, b0.1 100-20.degree. [bis-(phenylsemicarbazone), m. 229.degree. (from dioxane)] .lambda.max. in dioxane = 234 and 304 m.mu., log .epsilon., = 4.45 and 4.6, resp., orange-red color with $FeCl_3$. Pure trans-dihydrogeranic acid (9.0 g.) and 10 g. $SOCl_2$ after standing overnight and distg. gave the acid chloride, b12 88-90.degree.; to 30 g. in 40 cc. abs. Et_2O was added a soln. of $CdMe_2$ from 5 g. $CdCl_2$ and MeMgBr (from 1.2 g. Mg. and 5.0 g. MeBr) in abs. Et_2O during 40 min., the mixt. boiled 1.5 hrs., decompd. with ice and HCl, and extd. with Et_2O to give 1.9 g. methyl trans-2,2,6-trimethylcyclohexyl ketone (II), b12 86.degree. (no deriv. with semicarbazide or phenylsemicarbazide). II (1.9 g.) with 1.5 g. Ac_2O and BF_3 after 1 hr. gave 1.3 g. .beta.'-keto-trans-tetrahydroionone, b0.01 88.degree., .lambda.max. in alc. = 282 m.mu., log .epsilon. = 4.2 (monophenylsemicarbazone, m. 187-9.degree., .lambda.max. in alc. = 247 and 298 m.mu., log .epsilon. = 4.4 and 3.85, resp.). 3,4-Epoxy-.alpha.-ionone (III), b0.2 80.degree. (phenylsemicarbazone, m. 196.degree., .lambda.max. in alc. = 233 and 277 m.mu., log .epsilon. = 4.4 and 4.5, resp.), with Pd-$BaCO_3$ and H gave 3,4-epoxydihydro-.alpha.-ionone (IV), b0.1 78-91.degree., n_{22D} 1.4712 (phenylsemicarbazone, m. 167.degree., .lambda.max. in alc. = 248 m.mu., log .epsilon. = 4.4). After standing 3 days with 5 cc. 20% H_2SO_4 and 15 cc. alc., 0.5 g. IV gave a product $C_{13}H_{22}O_2$, b12 135.degree. (bath temp.), n_{22D} 1.4930 (strong $C(NO_2)_4$, but no carbonyl reactions), to which the cyclized structure 2,5,5,8a-tetramethyl-8-hydroxy-4a,5,6,7,8,8a-hexahydro-1,4H-benzopyran was given. IV (5 g.) in 20 cc. AcOH with 2 moles H and 0.4 g. PtO_2 gave a glassy residue, which in $CHCl_3$, treated with petr. ether till cloudy, gave 0.4 g. cryst. 4-ketotetrahydroionol (V), m. 129.degree., which also was obtained from III directly. V (0.10 g.) in 10 cc. AcOH with 0.10 g. CrO_3 in 10 cc. AcOH after standing overnight gave 4-ketotetrahydroionone (VI), b0.05 105.degree. (bath temp.) [bis(phenylsemicarbazone), m. 207-8.degree., .lambda.max. in dioxane = 247 m.mu., log .epsilon. = 4.8]; VI gave a large m.p. depression with I bis(phenylsemicarbazone). VI was also obtained from the noncryst. reduction product of V. Treatment of 0.45 g. VI with 1.0 g. $H_2NNH_2.H_2O$ and 0.7 g. Na in 15 cc. abs. EtOH 8 hrs. in a bomb tube at 200.degree. gave a hydrocarbon whose infrared spectrum is identical with that of authentic trans-tetrahydroionan. .alpha.',.beta.'-Epoxy-.alpha.-ionone (VII), m. 58.degree., (8 g.) (C.A. 41, 2017e) (phenylsemicarbazone, m. 176.degree. (from $CHCl_3$-MeOH), .lambda.max. in alc. = 253 m.mu., log .epsilon. = 4.25) with Pd-$BaCO_3$ and H absorbed 1 mole of H to give 3.1 g. colorless needles of .beta.'-hydroxydihydro-.alpha.-ionone (VIII), m. 63.degree. (from petr. ether), which gave no color with $FeCl_3$, a yellow with $C(NO_2)_4$ (phenylsemicarbazone (IX), m. 161.degree., .lambda.max. in alc. = 248, log .epsilon. = 4.45; 3,5-dinitrobenzoate, m. 138.degree. (from $CHCl_3$-MeOH)). VIII (0.5 g.) after 4 days in 5 cc. 20% H_2SO_4 and 15 cc. alc. gave .alpha.-ionone phenylsemicarbazone. Distn. of the oil from the reduction of VII gave .alpha.'-hydroxydihydro-.alpha.-ionone, b0.1 77-80.degree. (color with $FeCl_3$ and $C(NO_2)_4$) (phenylsemicarbazone, m. 171.degree., .lambda.max. in alc. = 253 m.mu., log .epsilon. = 4.45, gave a large depression of m.p. with

IX).

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	330.36	478.72

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-43.62	-43.62

STN INTERNATIONAL LOGOFF AT 12:04:42 ON 27 AUG 2003